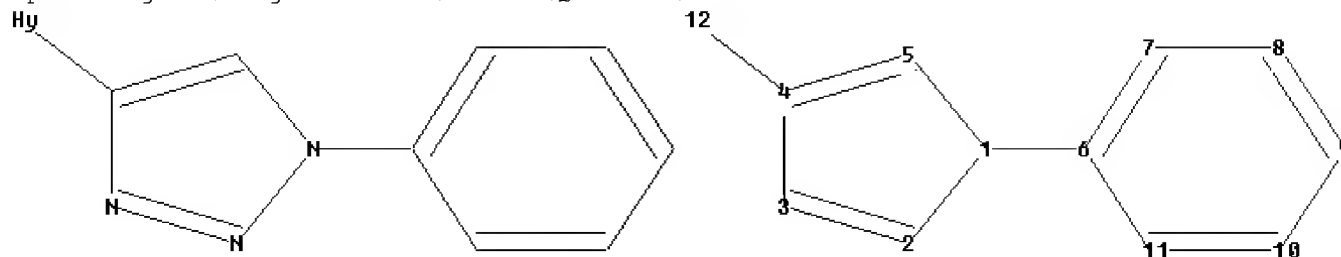


<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10590586A.str



chain nodes :

12

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-6 4-12

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 1-6 2-3 3-4 4-5 4-12

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom

Element Count :

Node 12: Limited

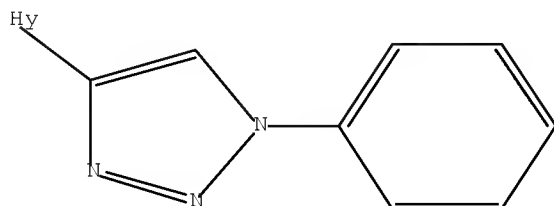
N,N1

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s sss sam l1

SAMPLE SEARCH INITIATED 17:02:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 9048 TO ITERATE

22.1% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

13 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 175258 TO 186662

PROJECTED ANSWERS: 716 TO 1636

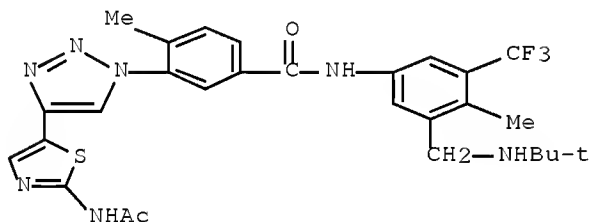
L2 13 SEA SSS SAM L1

=> d scan

L2 13 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzamide, 3-[4-[2-(acetylamino)-5-thiazolyl]-1H-1,2,3-triazol-1-yl]-N-[3-  
[[ (1,1-dimethylethyl)amino]methyl]-4-methyl-5-(trifluoromethyl)phenyl]-4-  
methyl-

MF C28 H30 F3 N7 O2 S



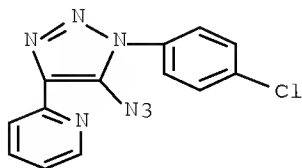
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L2 13 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

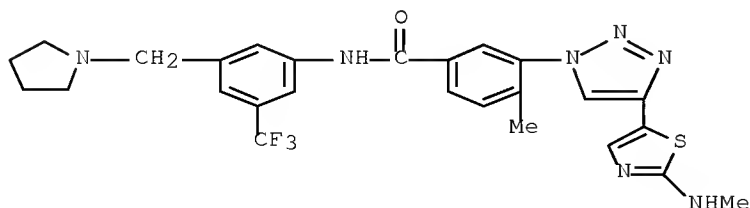
IN Pyridine, 2-[5-azido-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-

MF C13 H8 Cl N7



L2 13 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN Benzamide, 4-methyl-3-[4-[2-(methylamino)-5-thiazolyl]-1H-1,2,3-triazol-1-yl]-N-[3-(1-pyrrolidinylmethyl)-5-(trifluoromethyl)phenyl]-  
 MF C26 H26 F3 N7 O S

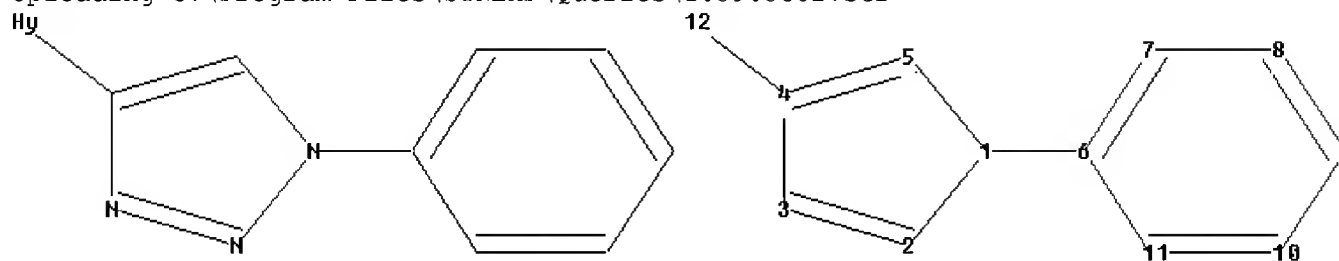


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=>

Uploading C:\Program Files\STNEXP\Queries\10590586B.str



chain nodes :

12

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-6 4-12

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-2 1-5 1-6 2-3 3-4 4-5 4-12

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom

Element Count :

Node 12: Limited

N,N1

S,S0

O,O0

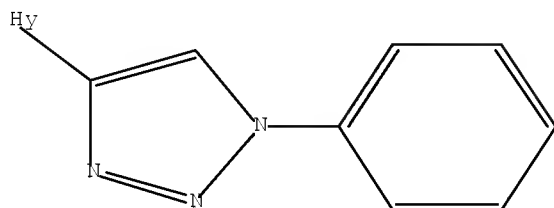
C,C5-9

L3 STRUCTURE UPLOADED

=> D L3

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> S SSS SAM

ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):END

SEARCH ENDED BY USER

=> S SSS SAM L3

SAMPLE SEARCH INITIATED 17:05:57 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 9048 TO ITERATE

22.1% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

6 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 175258 TO 186662

PROJECTED ANSWERS: 230 TO 854

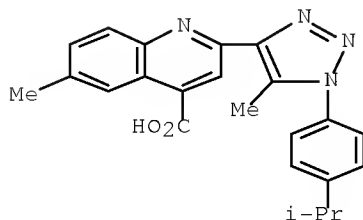
L4 6 SEA SSS SAM L3

=> D SCAN

L4 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 4-Quinolinecarboxylic acid, 6-methyl-2-[5-methyl-1-[4-(1-methylethyl)phenyl]-1H-1,2,3-triazol-4-yl]-

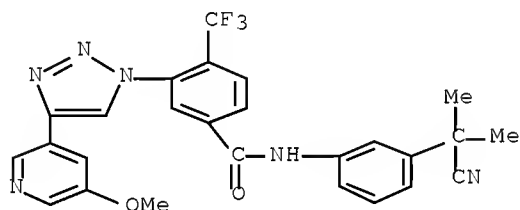
MF C23 H22 N4 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

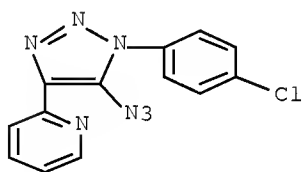
L4 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN Benzamide, N-[3-(1-cyano-1-methylethyl)phenyl]-3-[4-(5-methoxy-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-4-(trifluoromethyl)-  
MF C26 H21 F3 N6 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

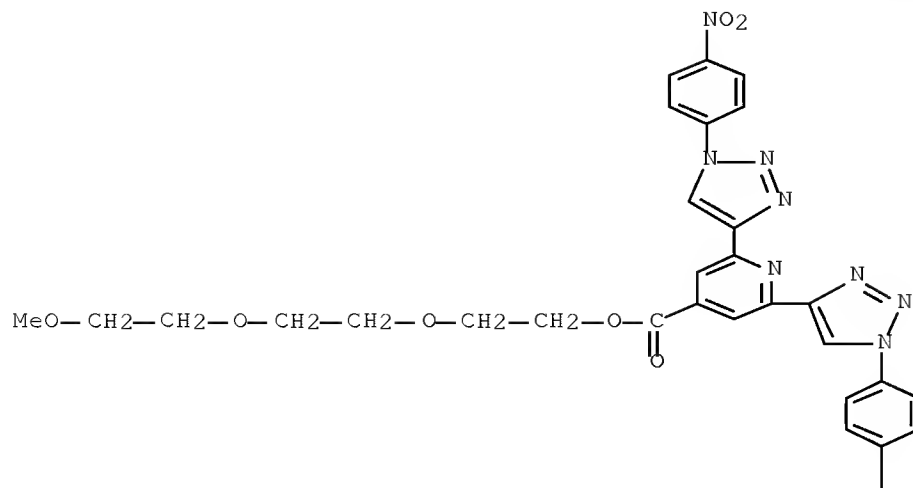
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L4 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN Pyridine, 2-[5-azido-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]-  
MF C13 H8 Cl N7



L4 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
IN 4-Pyridinecarboxylic acid, 2,6-bis[1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl]-, 2-[2-(2-methoxyethoxy)ethoxy]ethyl ester, compd. with dichloromethane (1:1)  
MF C29 H27 N9 O9 . C H2 Cl2

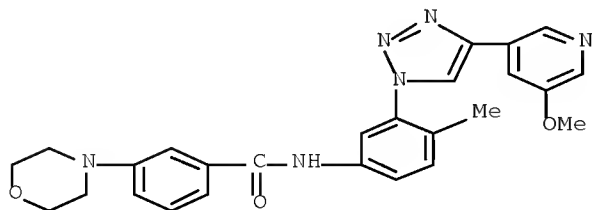
CM 1



CM 2



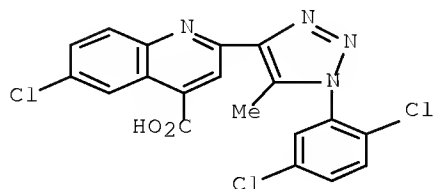
L4 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  
 IN Benzamide, N-[3-[4-(5-methoxy-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-4-methylphenyl]-3-(4-morpholinyl)-  
 MF C26 H26 N6 O3



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN 4-Quinolinecarboxylic acid, 6-chloro-2-[1-(2,5-dichlorophenyl)-5-methyl-1H-  
1,2,3-triazol-4-yl]-  
MF C19 H11 Cl3 N4 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> S SSS FULL L3

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 191.05 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y

FULL SEARCH INITIATED 17:06:43 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 183558 TO ITERATE

100.0% PROCESSED 183558 ITERATIONS

581 ANSWERS

SEARCH TIME: 00.00.15

L5 581 SEA SSS FUL L3

=> SAVE L5 HIRA10590586/A

ANSWER SET L5 HAS BEEN SAVED AS 'HIRA10590586/A'

=> FIL CAPLU

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

195.95

196.39

FILE 'CAPLUS' ENTERED AT 17:08:14 ON 11 MAR 2010

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FILE COVERS 1907 - 11 Mar 2010 VOL 152 ISS 11

FILE LAST UPDATED: 10 Mar 2010 (20100310/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

CAPLUS now includes complete International Patent Classification (IPC)  
reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

=> S L5

L6                    58 L5

=> S L6 AND (PY<2005 OR PRY<2005 OR AY<2005)

25157496 PY<2005

4640630 PRY<2005

5161844 AY<2005

L7                    17 L6 AND (PY<2005 OR PRY<2005 OR AY<2005)

=> E us 200!-590586/APPS

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E5                    1        US00-10056/AP

E6                    1        US00-10070/AP

E7                    1        US00-10178/AP

E8                    1        US00-10197/AP

E9                    3        US00-10220/AP

E10                   1        US00-102457/AP

E11                   1        US00-10268/AP

E12                   1        US00-103430/AP

=> E US200!-590586/APPS

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E3                    0 --> US200!-590586/AP

E4                    0        US200!-590586/PRN

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E6                    2        US2000-101566/AP

E7                    1        US2000-101862P/PRN

E8                    2        US2000-101907/PRN

E9                    1        US2000-102574/PRN

E10                   1        US2000-102914/AP

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=> S E3

L8 2 US2006-590586/AP

=> SEL RN L8

E1 THROUGH E557 ASSIGNED

=> FIL REG

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.94	209.33

FILE 'REGISTRY' ENTERED AT 17:12:41 ON 11 MAR 2010  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAR 2010 HIGHEST RN 1208531-15-0  
DICTIONARY FILE UPDATES: 10 MAR 2010 HIGHEST RN 1208531-15-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 8, 2010.

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> S E1-E557

1 100-46-9/BI  
(100-46-9/RN)

1 100-63-0/BI  
(100-63-0/RN)  
(994-89-8/RN)

1 99455-05-7/BI  
(99455-05-7/RN)

L9 557 (100-46-9/BI OR 100-63-0/BI OR 1003-03-8/BI OR 10075-50-0/BI OR  
100954-32-3/BI OR 102284-85-5/BI OR 102934-51-0/BI OR 10296-29-4  
/BI OR 104107-22-4/BI OR 107-10-8/BI OR 1072-97-5/BI OR 108281-7

=> D HIS

(FILE 'HOME' ENTERED AT 17:01:30 ON 11 MAR 2010)

FILE 'REGISTRY' ENTERED AT 17:02:23 ON 11 MAR 2010

L1 STRUCTURE UPLOADED

L2 13 S SSS SAM L1

```

L3          STRUCTURE UPLOADED
L4          6 S SSS SAM L3
L5          581 S SSS FULL L3
              SAVE L5 HIRA10590586/A

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FILE 'CAPLUS' ENTERED AT 17:08:14 ON 11 MAR 2010

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L6      58 S L5
L7      17 S L6 AND (PY<2005 OR PRY<2005 OR AY<2005)
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          E US200!-590586/APPS
          E US2006-590586/APPS
L8      2 S E3
          SEL RN L8

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FILE 'REGISTRY' ENTERED AT 17:12:41 ON 11 MAR 2010

L9 557 S E1-E557

=> S L9 AND L5

L10 74 L9 AND L5

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=> SAVE L10 TEMP HIR10590586/A
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ANSWER SET L10 HAS BEEN SAVED AS 'HIR10590586/A'

=> FIL CAPL

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

2.45

211.78

FILE 'CAPLUS' ENTERED AT 17:15:31 ON 11 MAR 2010

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FILE COVERS 1907 - 11 Mar 2010 VOL 152 ISS 11

FILE LAST UPDATED: 10 Mar 2010 (20100310/ED)

REVISÉD CLASS FIELDS (/NCL) LAST RELOADED: Dec 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S L10

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L11          4 L10

=> S L11 AND (PY<2005 OR PRY<2005 OR AY<2005)
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    4640630 PRY<2005
    5161844 AY<2005
L12          1 L11 AND (PY<2005 OR PRY<2005 OR AY<2005)

=> S L11 AND (PY<2006 OR PRY<2006 OR AY<2006)
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    5030714 PRY<2006
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=> D IBIB ABS HITST 1-2
'HITST' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

=> D HIS

      (FILE 'HOME' ENTERED AT 17:01:30 ON 11 MAR 2010)

      FILE 'REGISTRY' ENTERED AT 17:02:23 ON 11 MAR 2010
L1          STRUCTURE UPLOADED
L2          13 S SSS SAM L1
L3          STRUCTURE UPLOADED
L4          6 S SSS SAM L3
L5          581 S SSS FULL L3
            SAVE L5 HIRA10590586/A

      FILE 'CAPLUS' ENTERED AT 17:08:14 ON 11 MAR 2010
L6          58 S L5
L7          17 S L6 AND (PY<2005 OR PRY<2005 OR AY<2005)
            E US 200!-590586/APPS
            E US200!-590586/APPS
            E US2006-590586/APPS
L8          2 S E3
            SEL RN L8

      FILE 'REGISTRY' ENTERED AT 17:12:41 ON 11 MAR 2010
L9          557 S E1-E557
L10         74 S L9 AND L5
            SAVE L10 TEMP HIR10590586/A

      FILE 'CAPLUS' ENTERED AT 17:15:31 ON 11 MAR 2010
L11         4 S L10
L12         1 S L11 AND (PY<2005 OR PRY<2005 OR AY<2005)
L13         2 S L11 AND (PY<2006 OR PRY<2006 OR AY<2006)

=> D IBIB ABS HITS 1-2 L13
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DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):END

=> D IBIB ABS HITSTR 1-2
THE ESTIMATED COST FOR THIS REQUEST IS 11.62 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L13 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN

```

ACCESSION NUMBER: 2007:58485 CAPLUS Full-text  
 DOCUMENT NUMBER: 146:135605  
 TITLE: Combination drug containing diaryl-substituted  
 5-membered heterocyclic derivative  
 INVENTOR(S): Ohta, Hisashi; Sato, Akio; Kimura, Toshifumi; Suzuki,  
 Gentaroh; Kawamoto, Hiroshi  
 PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 56pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007007909	A1	20070118	WO 2006-JP314306	20060712 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: JP 2005-204526 A 20050713 <--  
 OTHER SOURCE(S): MARPAT 146:135605

AB A pharmaceutical comprising the combination of a diaryl-substituted 5-membered heterocyclic derivative having an mGluR1 inhibitory effect and one or more substances selected from the group consisting of (i) an mGluR1 inhibitor other than the derivative, (ii) an anticonvulsant, (iii) a therapeutic agent for an acute pain, an inflammatory pain or a chronic pain, (iv) a therapeutic agent for a brain disorder such as cerebral infarction or transient ischemic attack, (v) a therapeutic agent for schizophrenia, (vi) an antianxiety agent, (vii) a therapeutic agent for drug dependence, (viii) a therapeutic agent for Parkinson's disease and (ix) a therapeutic agent for a gastrointestinal disorder.

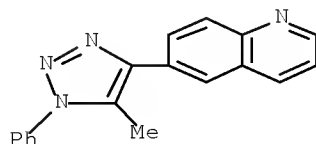
IT 864863-68-3P 864864-86-8P 864865-16-7P  
 864865-43-0P 864865-47-4P 864865-70-3P  
 864865-90-7P 864865-93-0P 864873-71-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

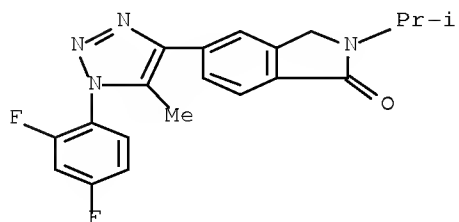
(combination drug containing diaryl-substituted 5-membered heterocyclic derivs. for treatment of brain diseases, drug dependence, and gastrointestinal disorder)

RN 864863-68-3 CAPLUS

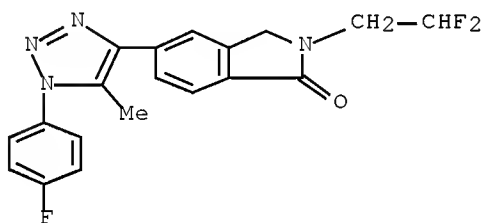
CN Quinoline, 6-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



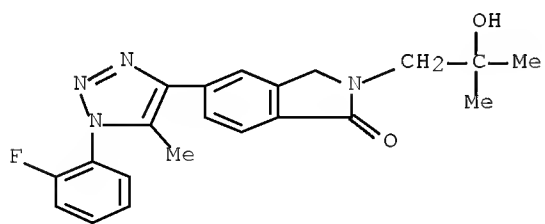
RN 864864-86-8 CAPLUS  
 CN 1H-Isoindol-1-one, 5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(1-methylethyl)- (CA INDEX NAME)



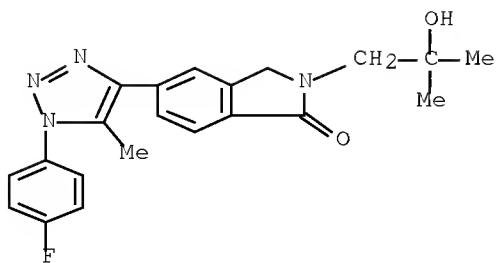
RN 864865-16-7 CAPLUS  
 CN 1H-Isoindol-1-one, 2-(2,2-difluoroethyl)-5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



RN 864865-43-0 CAPLUS  
 CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(2-hydroxy-2-methylpropyl)- (CA INDEX NAME)

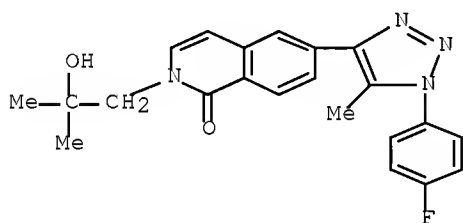


RN 864865-47-4 CAPLUS  
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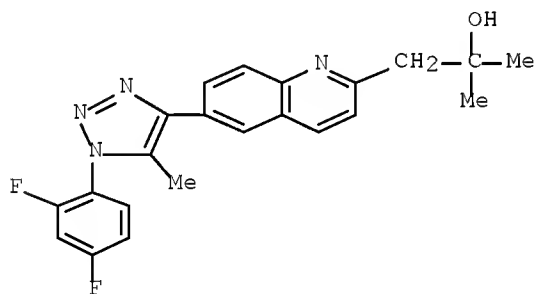
RN 864865-70-3 CAPLUS

CN 1(2H)-Isoquinolinone, 6-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2-(2-hydroxy-2-methylpropyl)- (CA INDEX NAME)



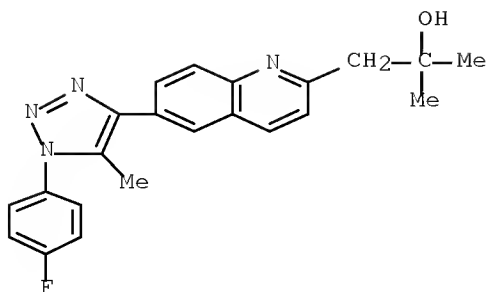
RN 864865-90-7 CAPLUS

CN 2-Quinolineethanol, 6-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-α,α-dimethyl- (CA INDEX NAME)

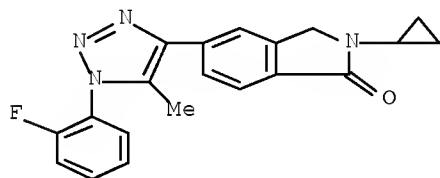


RN 864865-93-0 CAPLUS

CN 2-Quinolineethanol, 6-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-α,α-dimethyl- (CA INDEX NAME)



RN 864873-71-2 CAPLUS  
 CN 1H-Isoindol-1-one, 2-cyclopropyl-5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

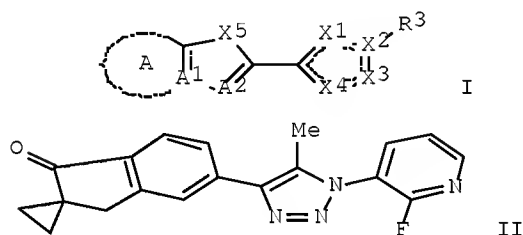
L13 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN  
 ACCESSION NUMBER: 2005:1004722 CAPLUS Full-text  
 DOCUMENT NUMBER: 143:306320  
 TITLE: Preparation of diaryl-substituted triazole derivatives as mGluR1 inhibitors  
 INVENTOR(S): Kawamoto, Hiroshi; Ito, Satoru; Satoh, Atsushi; Nagatomi, Yasushi; Hirata, Yukari; Kimura, Toshifumi; Suzuki, Gentaroh; Sato, Akio; Ohta, Hisashi  
 PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd, Japan  
 SOURCE: PCT Int. Appl., 323 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085214	A1	20050915	WO 2005-JP4379	20050307 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, BG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,				

MR, NE, SN, TD, TG

AU 2005219791	A1	20050915	AU 2005-219791	20050307 <--
CA 2558278	A1	20050915	CA 2005-2558278	20050307 <--
EP 1726585	A1	20061129	EP 2005-720650	20050307 <--
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IN 2006DN04785	A	20070831	IN 2006-DN4785	20060821 <--
US 20070173507	A1	20070726	US 2006-590586	20060824 <--
PRIORITY APPLN. INFO.:			JP 2004-63243	A 20040305 <--
			WO 2005-JP4379	W 20050307 <--

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT  
 OTHER SOURCE(S): MARPAT 143:306320  
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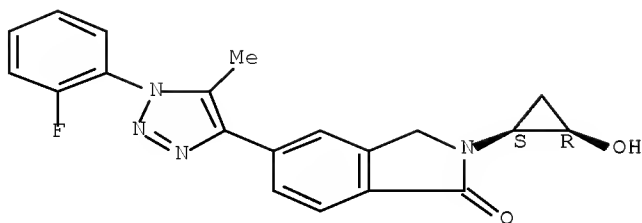
AB Title compds. represented by the formula I [wherein X1 = O, N or CR2; X2-X4, A1 = independently N or C; X5 = S or A4:A3; A2-A4 = independently CR4 or N; ring A = (hetero)cyclcyl or (hetero)aryl; R2 = H, alkyl, cyano, alkyloxy(carbonyl) or trialkylsilyl; R4 = H, halo, alkyl(oxy), etc.; R3 = halo, alkyl(oxy), cyano, etc.; and pharmaceutically acceptable salts thereof] were prepared as mGluR1 (metabotropic Glutamate receptor 1) inhibitors. For example, II was given in a multi-step synthesis starting from 5-bromoindanone. II showed inhibition of mGluR1a with an IC50 value of 2.3 nM. Thus, I are useful for the prevention or treatment of convulsion, acute pains, inflammatory pains, chronic pains, brain disorders such as brain infarction or transient cerebral ischemic attack, mental function disorders such as schizophrenia, anxiety, drug dependence, Parkinson's disease, or gastrointestinal disorders (no data).

IT 864865-07-6P 864865-17-8P 864866-07-9P  
 864866-08-0P  
 RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of diaryl-substituted triazole derivs. as mGluR1 inhibitors)

RN 864865-07-6 CAPLUS  
 CN 1H-Isoidol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-[(1R,2S)-2-hydroxycyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

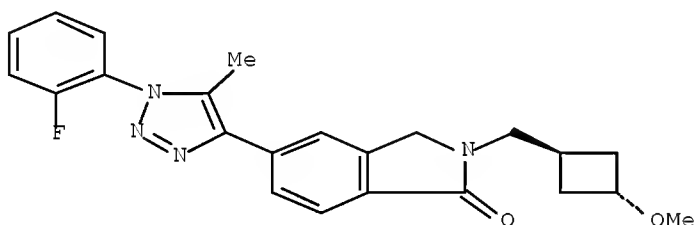




RN 864865-17-8 CAPLUS

CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-[(trans-3-methoxycyclobutyl)methyl]- (CA INDEX NAME)

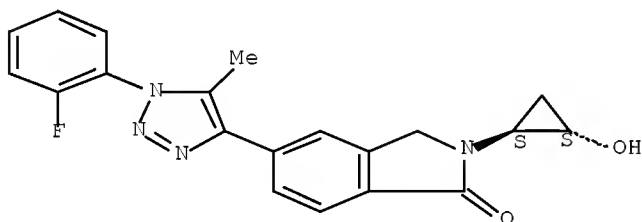
Relative stereochemistry.



RN 864866-07-9 CAPLUS

CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-[(1R,2R)-2-hydroxycyclopropyl]-, rel- (CA INDEX NAME)

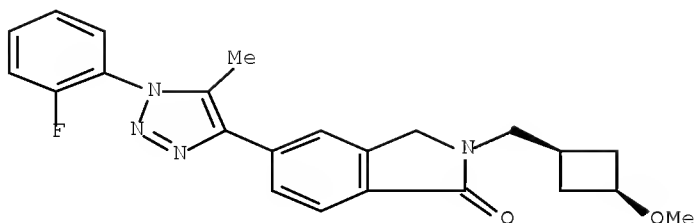
Relative stereochemistry.



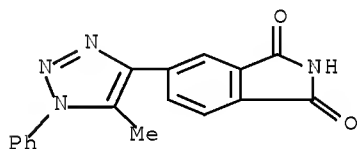
RN 864866-08-0 CAPLUS

CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-[(cis-3-methoxycyclobutyl)methyl]- (CA INDEX NAME)

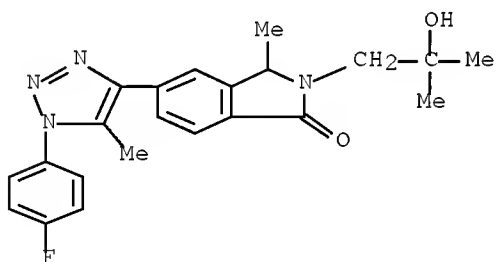
Relative stereochemistry.



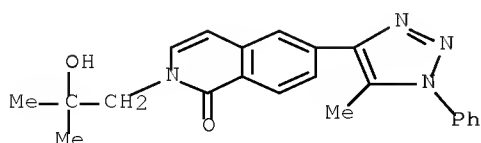
IT 864863-78-5P 864865-83-8P 864865-85-0P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of diaryl-substituted triazole derivs. as mGluR1 inhibitors)  
 RN 864863-78-5 CAPLUS  
 CN 1H-Isoindole-1,3(2H)-dione, 5-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)-  
 (CA INDEX NAME)



RN 864865-83-8 CAPLUS  
 CN 1H-Isoindol-1-one, 5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-  
 2,3-dihydro-2-(2-hydroxy-2-methylpropyl)-3-methyl- (CA INDEX NAME)



RN 864865-85-0 CAPLUS  
 CN 1(2H)-Isoquinolinone, 2-(2-hydroxy-2-methylpropyl)-6-(5-methyl-1-phenyl-1H-  
 1,2,3-triazol-4-yl)- (CA INDEX NAME)



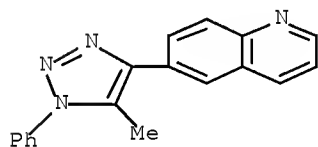
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	864865-12-3P	864865-13-4P	864865-14-5P
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	864865-82-7P	864865-84-9P	864865-86-1P
	864865-88-3P	864865-89-4P	864865-90-7P
	864865-91-8P	864865-93-0P	864865-94-1P
	864873-71-2P		

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryl-substituted triazole derivs. as mGluR1 inhibitors)

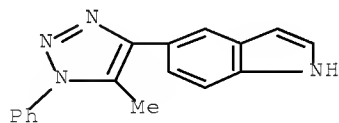
RN 864863-68-3 CAPLUS

CN Quinoline, 6-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



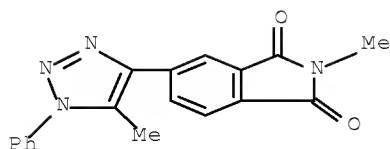
RN 864863-71-8 CAPLUS

CN 1H-Indole, 5-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



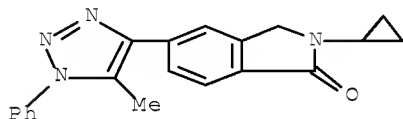
RN 864863-79-6 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-methyl-5-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



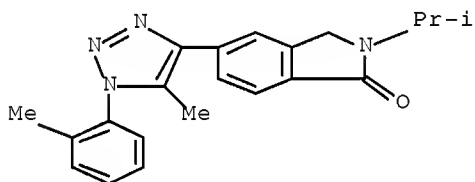
RN 864864-59-5 CAPLUS

CN 1H-Isoindol-1-one, 2-cyclopropyl-2,3-dihydro-5-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



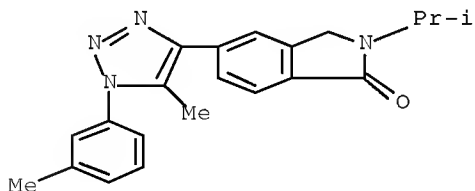
RN 864864-79-9 CAPLUS

CN 1H-Isoindol-1-one, 2,3-dihydro-2-(1-methylethyl)-5-[5-methyl-1-(2-methylphenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



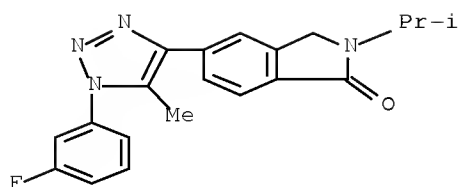
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CN 1H-Isoindol-1-one, 2,3-dihydro-2-(1-methylethyl)-5-[5-methyl-1-(3-methylphenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)

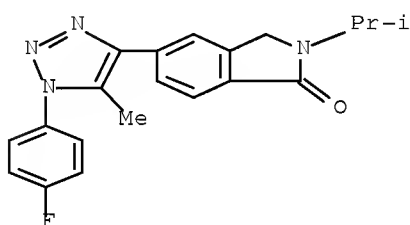


RN 864864-81-3 CAPLUS

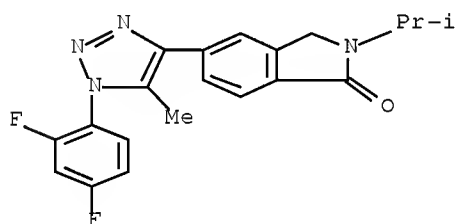
CN 1H-Isoindol-1-one, 5-[1-(3-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(1-methylethyl)- (CA INDEX NAME)



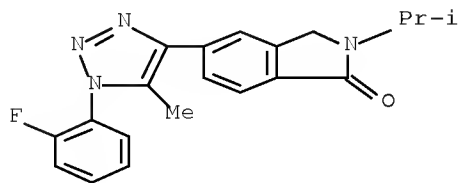
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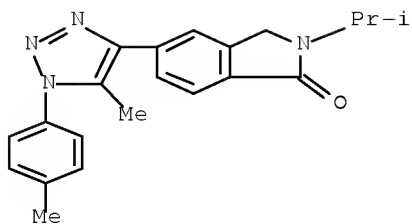
RN 864864-86-8 CAPLUS  
 CN 1H-Isoindol-1-one, 5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(1-methylethyl)- (CA INDEX NAME)



RN 864864-87-9 CAPLUS  
 CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(1-methylethyl)- (CA INDEX NAME)

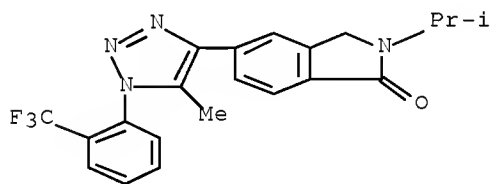


RN 864864-90-4 CAPLUS  
 CN 1H-Isoindol-1-one, 2,3-dihydro-2-(1-methylethyl)-5-[5-methyl-1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



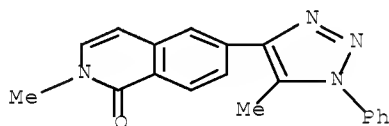
RN 864864-92-6 CAPLUS

CN 1H-Isoindol-1-one, 2,3-dihydro-2-(1-methylethyl)-5-[5-methyl-1-[2-(trifluoromethyl)phenyl]-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



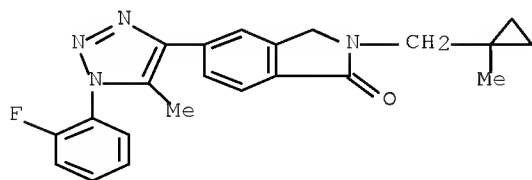
RN 864864-94-8 CAPLUS

CN 1(2H)-Isoquinolinone, 2-methyl-6-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



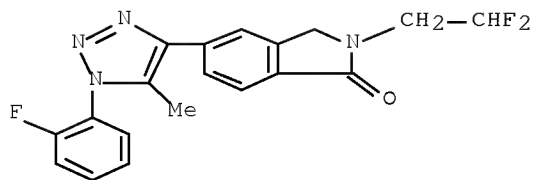
RN 864865-09-8 CAPLUS

CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-[(1-methylcyclopropyl)methyl]- (CA INDEX NAME)



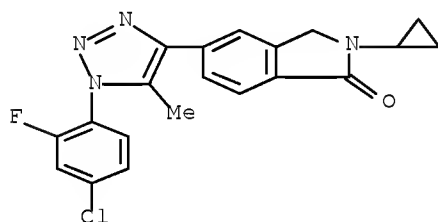
RN 864865-11-2 CAPLUS

CN 1H-Isoindol-1-one, 2-(2,2-difluoroethyl)-5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



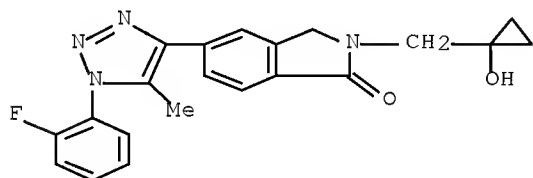
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CN 1H-Isoindol-1-one, 5-[1-(4-chloro-2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2-cyclopropyl-2,3-dihydro- (CA INDEX NAME)



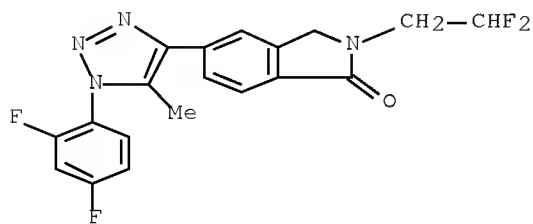
RN 864865-13-4 CAPLUS

CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-[(1-hydroxycyclopropyl)methyl]- (CA INDEX NAME)



RN 864865-14-5 CAPLUS

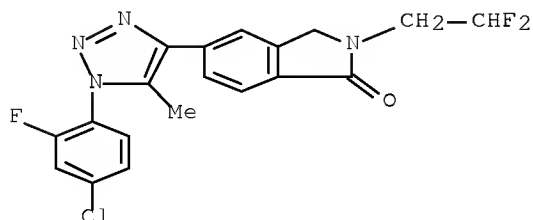
CN 1H-Isoindol-1-one, 2-(2,2-difluoroethyl)-5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



RN 864865-15-6 CAPLUS

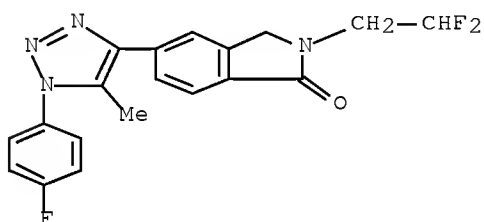
CN 1H-Isoindol-1-one, 5-[1-(4-chloro-2-fluorophenyl)-5-methyl-1H-1,2,3-

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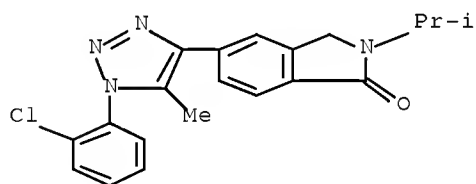
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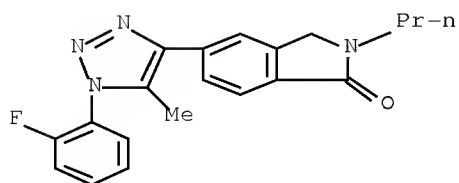
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CN 1H-Isoindol-1-one, 5-[1-(2-chlorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(1-methylethyl)- (CA INDEX NAME)



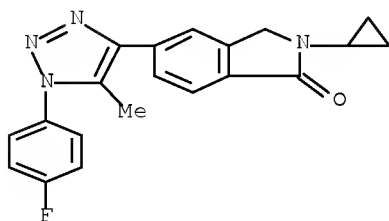
RN 864865-19-0 CAPLUS

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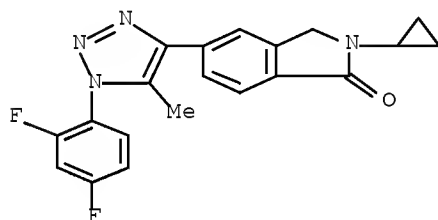




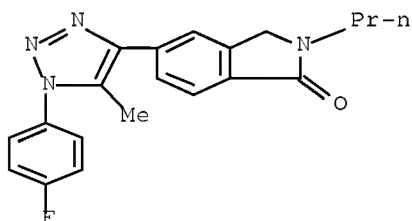
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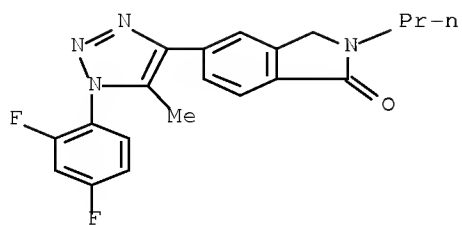
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 CN 1H-Isoindol-1-one, 2-cyclopropyl-5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



RN 864865-22-5 CAPLUS  
 CN 1H-Isoindol-1-one, 5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-propyl- (CA INDEX NAME)

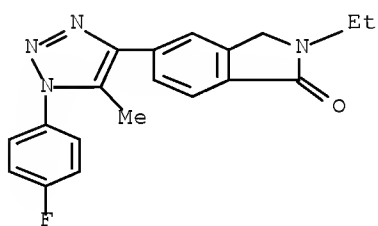


RN 864865-23-6 CAPLUS  
 CN 1H-Isoindol-1-one, 5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-propyl- (CA INDEX NAME)



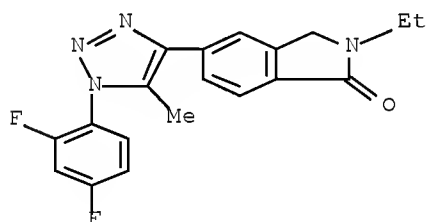
RN 864865-25-8 CAPLUS

CN 1H-Isoindol-1-one, 2-ethyl-5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



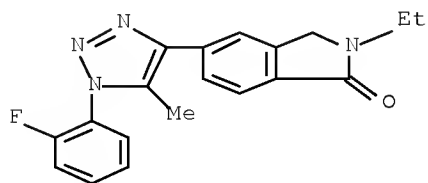
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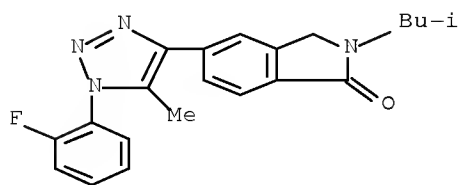
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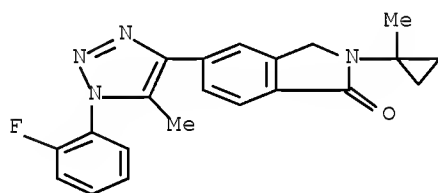
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CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-  
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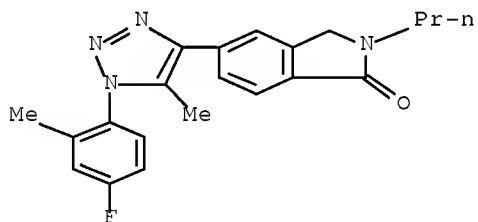
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CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-  
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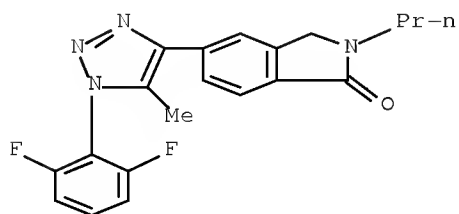
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CN 1H-Isoindol-1-one, 5-[1-(4-fluoro-2-methylphenyl)-5-methyl-1H-1,2,3-  
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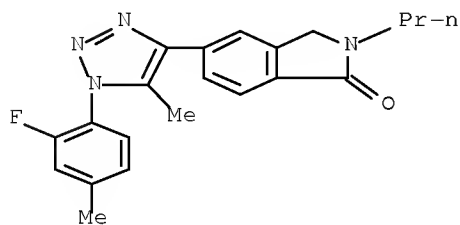


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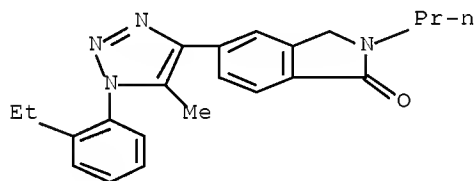
CN 1H-Isoindol-1-one, 5-[1-(2,6-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-  
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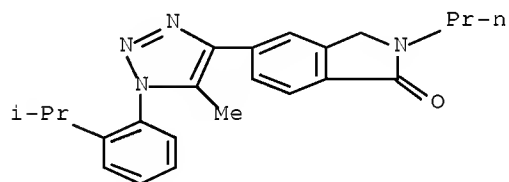
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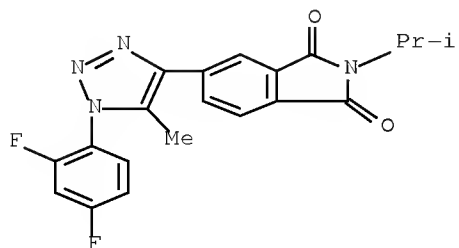
RN 864865-38-3 CAPLUS  
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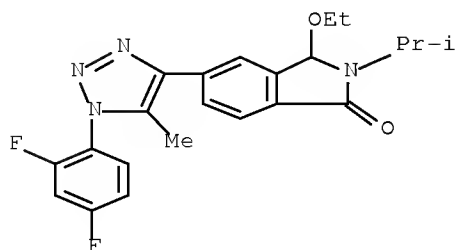
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 CN 1H-Isoindol-1-one, 2,3-dihydro-5-[5-methyl-1-[2-(1-methylethyl)phenyl]-1H-1,2,3-triazol-4-yl]-2-propyl- (CA INDEX NAME)



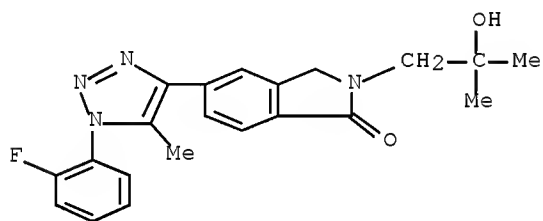
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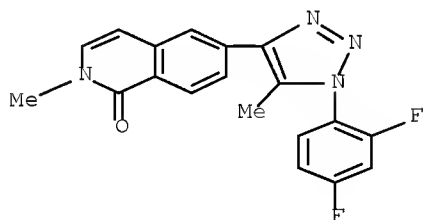
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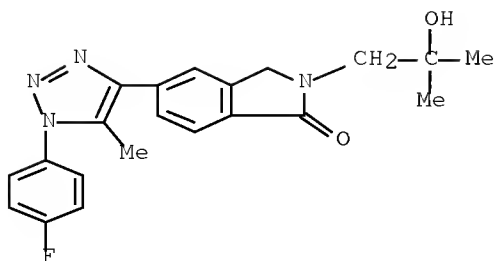
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 CN 1H-Isoindol-1-one, 5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(2-hydroxy-2-methylpropyl)- (CA INDEX NAME)



RN 864865-45-2 CAPLUS  
 CN 1(2H)-Isoquinolinone, 6-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2-methyl- (CA INDEX NAME)

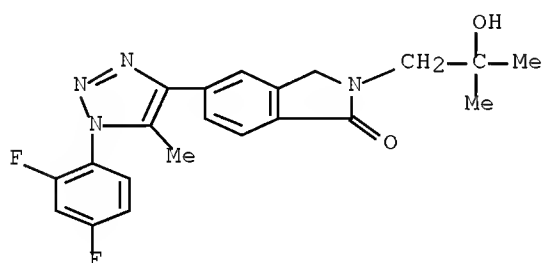


RN 864865-47-4 CAPLUS  
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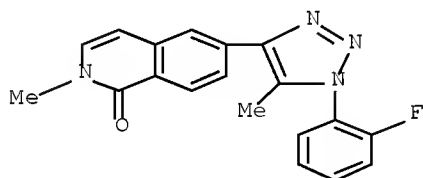
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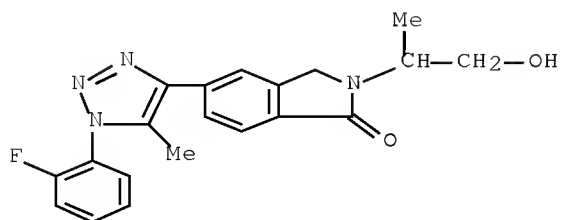
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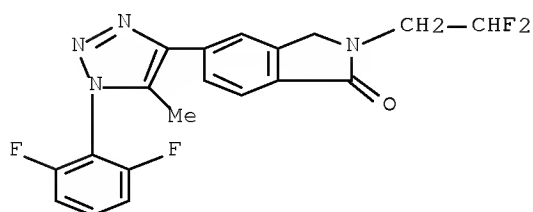


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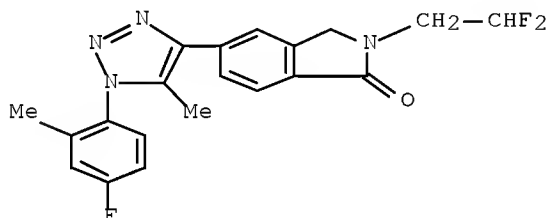
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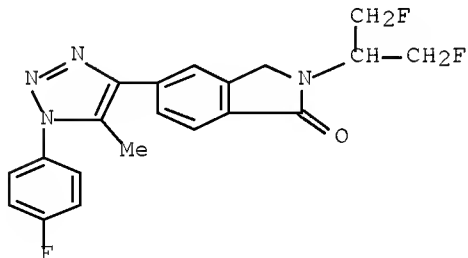
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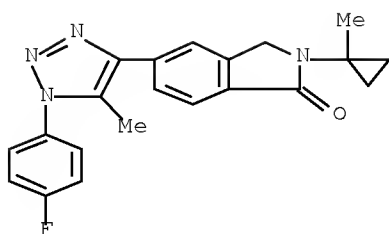
RN 864865-58-7 CAPLUS  
 CN 1H-Isoindol-1-one, 2-(2,2-difluoroethyl)-5-[1-(4-fluoro-2-methylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



RN 864865-62-3 CAPLUS  
 CN 1H-Isoindol-1-one, 2-[2-fluoro-1-(fluoromethyl)ethyl]-5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)

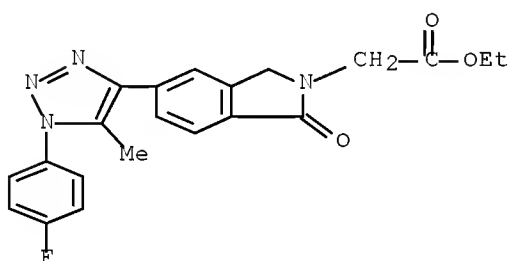


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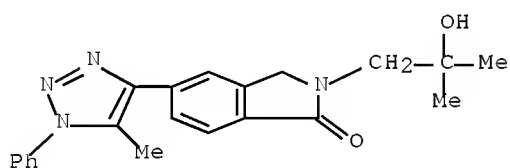
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CN 2H-Isoindole-2-acetic acid, 5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-1,3-dihydro-1-oxo-, ethyl ester (CA INDEX NAME)



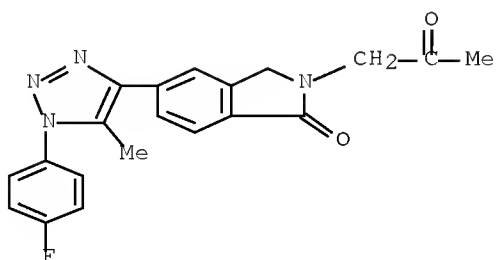
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CN 1H-Isoindol-1-one, 2,3-dihydro-2-(2-hydroxy-2-methylpropyl)-5-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



RN 864865-69-0 CAPLUS

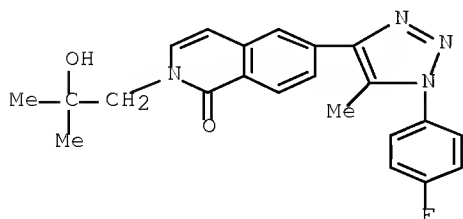
CN 1H-Isoindol-1-one, 5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(2-oxopropyl)- (CA INDEX NAME)





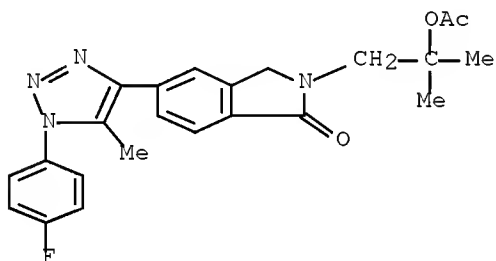
RN 864865-70-3 CAPLUS

CN 1(2H)-Isoquinolinone, 6-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2-(2-hydroxy-2-methylpropyl)- (CA INDEX NAME)



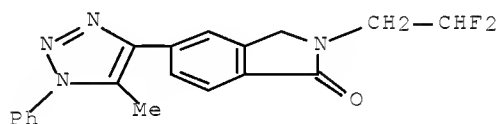
RN 864865-71-4 CAPLUS

CN 1H-Isoindol-1-one, 2-[2-(acetyloxy)-2-methylpropyl]-5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



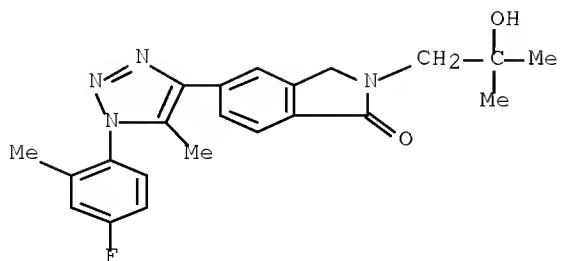
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CN 1H-Isoindol-1-one, 2-(2,2-difluoroethyl)-2,3-dihydro-5-(5-methyl-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



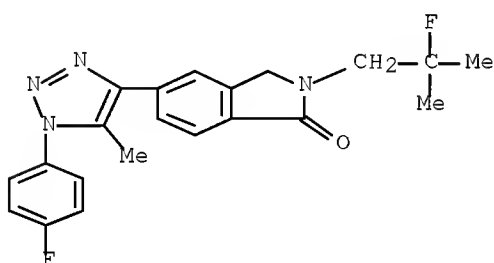
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CN 1H-Isoindol-1-one, 5-[1-(4-fluoro-2-methylphenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(2-hydroxy-2-methylpropyl)- (CA INDEX NAME)



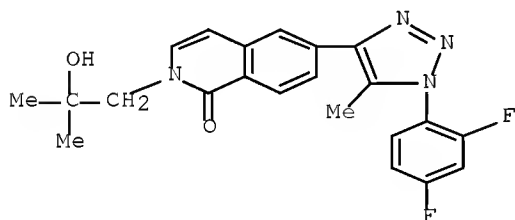
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CN 1H-Isoindol-1-one, 2-(2-fluoro-2-methylpropyl)-5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



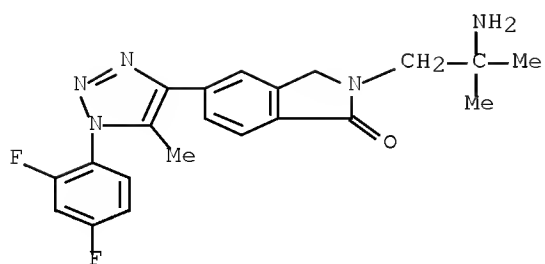
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CN 1(2H)-Isoquinolinone, 6-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2-(2-hydroxy-2-methylpropyl)- (CA INDEX NAME)



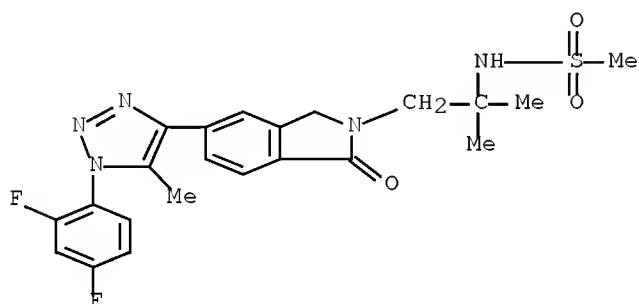
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CN 1H-Isoindol-1-one, 2-(2-amino-2-methylpropyl)-5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



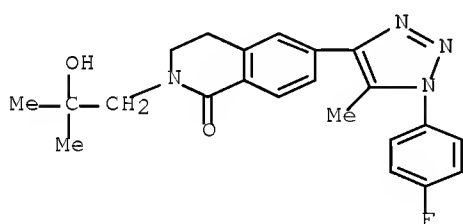
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CN Methanesulfonamide, N-[2-[5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-1,3-dihydro-1-oxo-2H-isoindol-2-yl]-1,1-dimethylethyl]- (CA INDEX NAME)



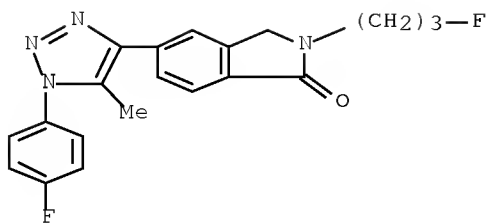
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CN 1(2H)-Isoquinolinone, 6-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-3,4-dihydro-2-(2-hydroxy-2-methylpropyl)- (CA INDEX NAME)



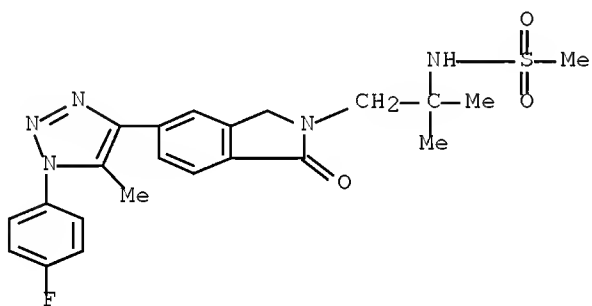
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CN 1H-Isoindol-1-one, 5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2-(3-fluoropropyl)-2,3-dihydro- (CA INDEX NAME)



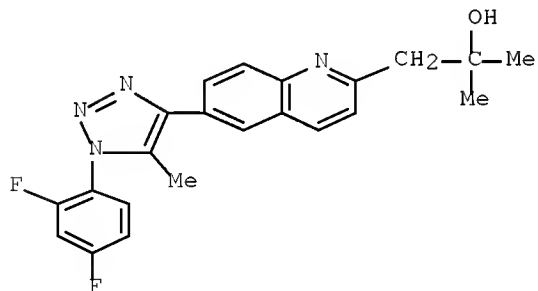
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CN Methanesulfonamide, N-[2-[5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-1,3-dihydro-1-oxo-2H-isoindol-2-yl]-1,1-dimethylethyl]- (CA INDEX NAME)



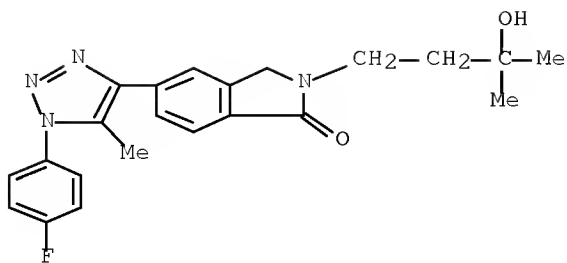
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CN 2-Quinolineethanol, 6-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]- $\alpha,\alpha$ -dimethyl- (CA INDEX NAME)



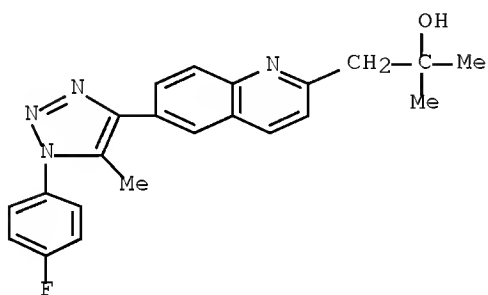
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CN 1H-Isoindol-1-one, 5-[1-(4-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro-2-(3-hydroxy-3-methylbutyl)- (CA INDEX NAME)



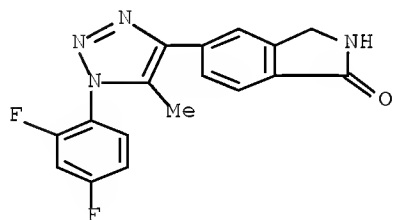
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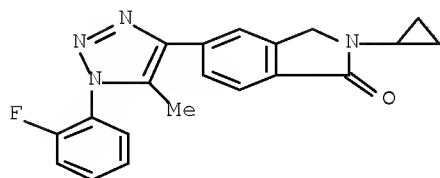
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CN 1H-Isoindol-1-one, 5-[1-(2,4-difluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



RN 864873-71-2 CAPLUS

CN 1H-Isoindol-1-one, 2-cyclopropyl-5-[1-(2-fluorophenyl)-5-methyl-1H-1,2,3-triazol-4-yl]-2,3-dihydro- (CA INDEX NAME)



OS.CITING REF COUNT: 9 THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD  
(9 CITINGS)  
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 17:01:30 ON 11 MAR 2010)

FILE 'REGISTRY' ENTERED AT 17:02:23 ON 11 MAR 2010

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L2 13 S SSS SAM L1  
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L4 6 S SSS SAM L3  
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FILE 'CAPLUS' ENTERED AT 17:08:14 ON 11 MAR 2010

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THE ESTIMATED COST FOR THIS REQUEST IS 92.96 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L15 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2006:446018 CAPLUS Full-text  
DOCUMENT NUMBER: 144:468176

L15 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 2005:1042236 CAPLUS Full-text  
DOCUMENT NUMBER: 143:347181  
TITLE: Preparation of triazolyl arylbenzamides as inhibitors

of cytokines  
INVENTOR(S): Cogan, Derek; Hao, Ming-Hong; Kamhi, Victor Marc;  
Miller, Craig Andrew; Netherton, Matthew Russell;  
Swinamer, Alan David  
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA  
SOURCE: PCT Int. Appl., 226 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090333	A1	20050929	WO 2005-US6997	20050304 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005223738	A1	20050929	AU 2005-223738	20050304 <--
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EP 1725544	B1	20090527		
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BA, HR, LV, YU				
CN 1930144	A	20070314	CN 2005-80007873	20050304 <--
BR 2005008561	A	20070814	BR 2005-8561	20050304 <--
JP 2007528395	T	20071011	JP 2007-502866	20050304 <--
EP 1887003	A1	20080213	EP 2007-112458	20050304 <--
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BA, HR, LV, YU				
AT 432273	T	20090615	AT 2005-724523	20050304 <--
ES 2327940	T3	20091105	ES 2005-724523	20050304 <--
US 20060079519	A1	20060413	US 2005-74354	20050307 <--
US 7214802	B2	20070508		
ZA 2006006177	A	20081231	ZA 2006-6177	20060726 <--
MX 2006010235	A	20061030	MX 2006-10235	20060908 <--
NO 2006004120	A	20060926	NO 2006-4120	20060913 <--
KR 2006129077	A	20061214	KR 2006-720618	20061002 <--
US 20070142371	A1	20070621	US 2007-668704	20070130 <--
US 7514458	B2	20090407		
PRIORITY APPLN. INFO.:			US 2004-551445P	P 20040309 <--
			EP 2005-724523	A3 20050304
			WO 2005-US6997	W 20050304
			US 2005-74354	A3 20050307

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 143:347181; MARPAT 143:347181

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

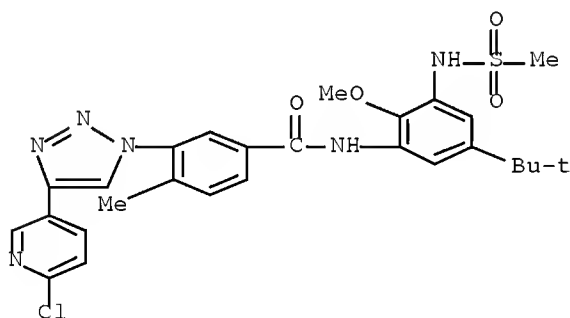
AB Title compds. I [Arl = substituted carbocycle, heteroaryl or benzofused heterocyclic ring; D, A, and B independently = H or CH wherein the hydrogen atom is optionally displaced by R3; Het = (un)substituted heterocycle or heteroaryl; R1, R2 and R3 independently = H, halo, OH, etc.; X = O or S] and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of cytokines. Thus, e.g., II was prepared by cyclization of 2-chloro-5-ethynylpyridine (preparation given) with 3-azido-4-Me benzoic acid followed by coupling with N-(3-amino-5-tert-butyl-2-methoxy-phenyl)-methane-sulfonamide. The activity of I was evaluated by measuring the inhibition of TNF $\alpha$  in liposaccharide stimulated THP cells and preferred compds. have an IC50 below 1  $\mu$ M in this assay (no data). I as inhibitors of cytokines should prove useful in the treatment of diseases such as but not limited to osteoarthritis, atherosclerosis and contact dermatitis. Pharmaceutical compns. comprising I are disclosed.

IT 865796-09-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of triazolyl arylbenzamides as inhibitors of cytokines)

RN 865796-09-4 CAPLUS

CN Benzamide, 3-[4-(6-chloro-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (CA INDEX NAME)



IT 865796-11-8P 865796-13-0P 865796-15-2P  
865796-17-4P 865796-18-5P 865796-19-6P  
865796-20-9P 865796-21-0P 865796-22-1P  
865796-23-2P 865796-24-3P 865796-25-4P  
865796-26-5P 865796-27-6P 865796-28-7P  
865796-29-8P 865796-31-2P 865796-32-3P  
865796-33-4P 865796-34-5P 865796-35-6P  
865796-36-7P 865796-38-9P 865796-40-3P  
865796-50-5P 865796-83-4P 865797-72-4P  
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865798-01-2P

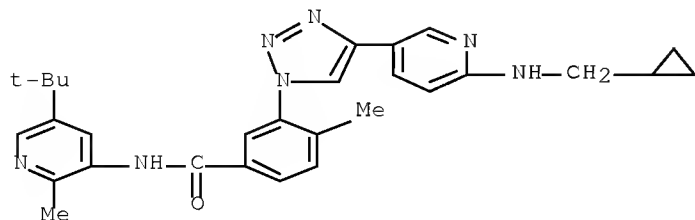
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of triazolyl arylbenzamides as inhibitors of cytokines)

RN 865796-11-8 CAPLUS

CN Benzamide, 3-[4-[6-[(cyclopropylmethyl)amino]-3-pyridinyl]-1H-1,2,3-

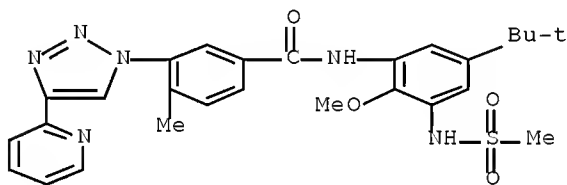


triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methyl-3-pyridinyl]-4-methyl-  
(CA INDEX NAME)



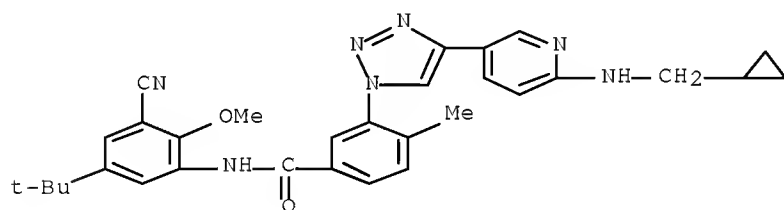
RN 865796-13-0 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-  
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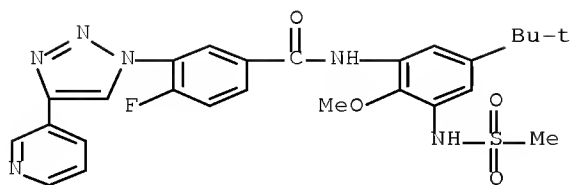
RN 865796-15-2 CAPLUS

CN Benzamide, N-[3-cyano-5-(1,1-dimethylethyl)-2-methoxyphenyl]-3-[4-[6-  
[(cyclopropylmethyl)amino]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-4-methyl-  
(CA INDEX NAME)



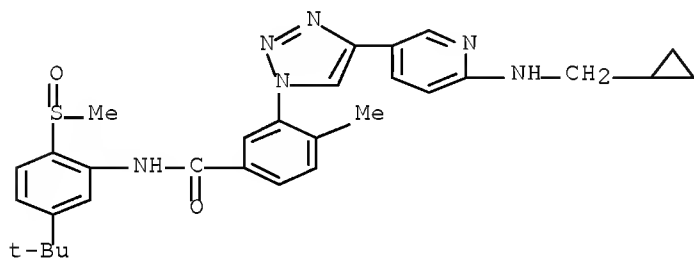
RN 865796-17-4 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-  
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triazol-1-yl]- (CA INDEX NAME)



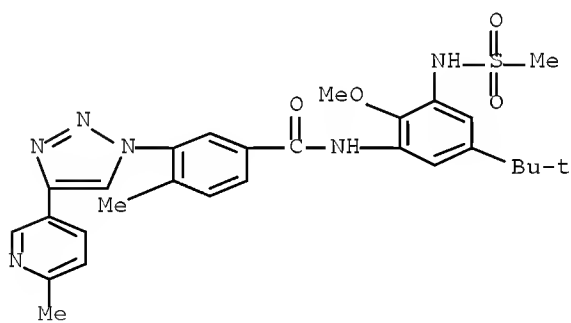
RN 865796-18-5 CAPLUS

CN Benzamide, 3-[4-[6-[(cyclopropylmethyl)amino]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-(methylsulfinyl)phenyl]-4-methyl- (CA INDEX NAME)



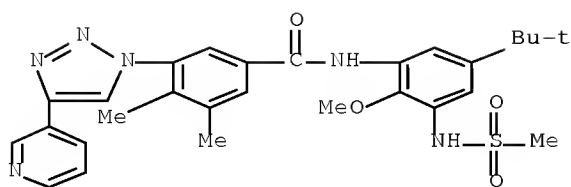
RN 865796-19-6 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-(6-methyl-3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



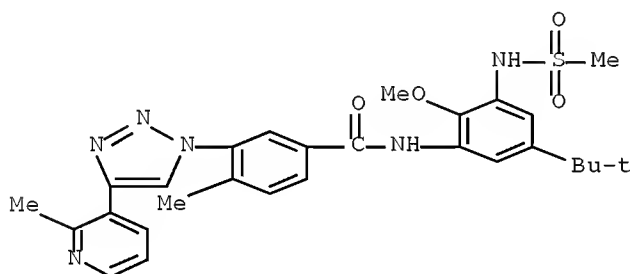
RN 865796-20-9 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-3,4-dimethyl-5-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



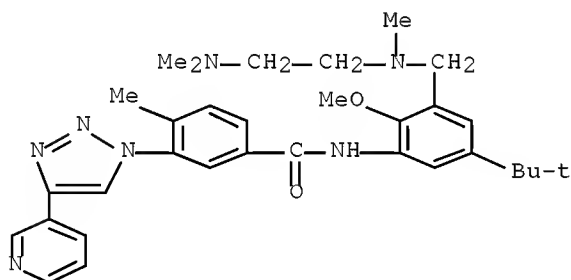
RN 865796-21-0 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-(2-methyl-3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



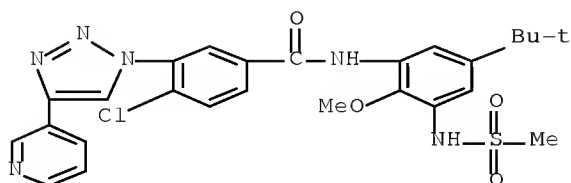
RN 865796-22-1 CAPLUS

CN Benzamide, N-[3-[[[2-(dimethylamino)ethyl]methylamino]methyl]-5-(1,1-dimethylethyl)-2-methoxyphenyl]-4-methyl-3-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



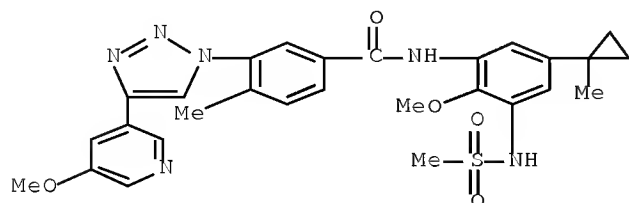
RN 865796-23-2 CAPLUS

CN Benzamide, 4-chloro-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-3-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



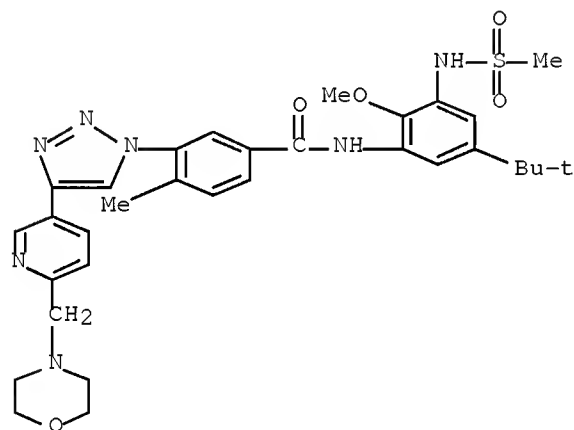
RN 865796-24-3 CAPLUS

CN Benzamide, N-[2-methoxy-5-(1-methylcyclopropyl)-3-[(methylsulfonyl)amino]phenyl]-3-[4-(5-methoxy-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-4-methyl- (CA INDEX NAME)



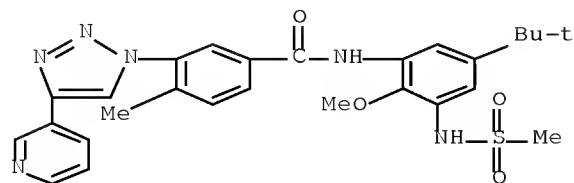
RN 865796-25-4 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



RN 865796-26-5 CAPLUS

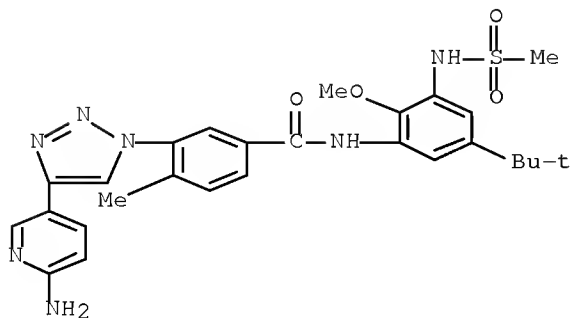
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



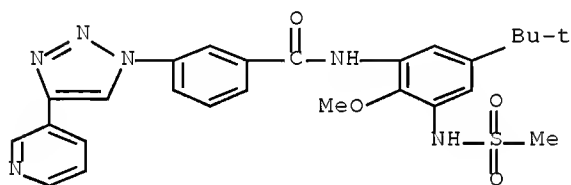
RN 865796-27-6 CAPLUS

CN Benzamide, 3-[4-(6-amino-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-

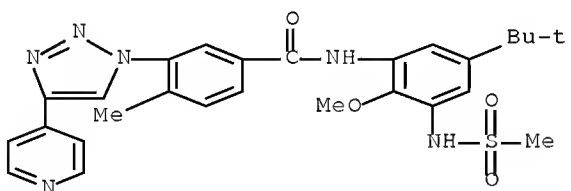
dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (CA  
INDEX NAME)



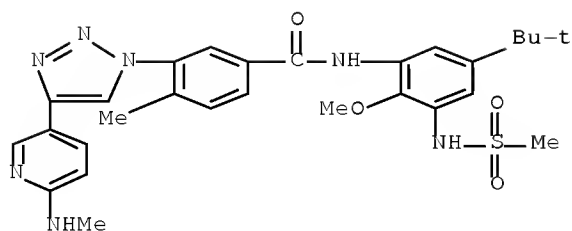
RN 865796-28-7 CAPLUS  
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-  
[(methylsulfonyl)amino]phenyl]-3-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]-  
(CA INDEX NAME)



RN 865796-29-8 CAPLUS  
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-  
[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-(4-pyridinyl)-1H-1,2,3-  
triazol-1-yl]- (CA INDEX NAME)

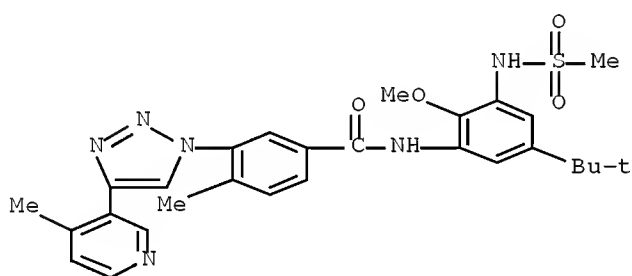


RN 865796-31-2 CAPLUS  
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-  
[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-[6-(methylamino)-3-pyridinyl]-  
1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



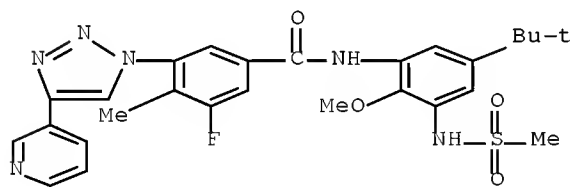
RN 865796-32-3 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-(4-methyl-3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



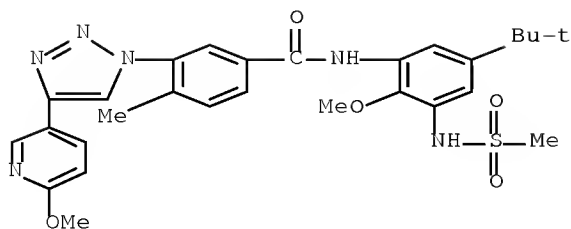
RN 865796-33-4 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-3-fluoro-4-methyl-5-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



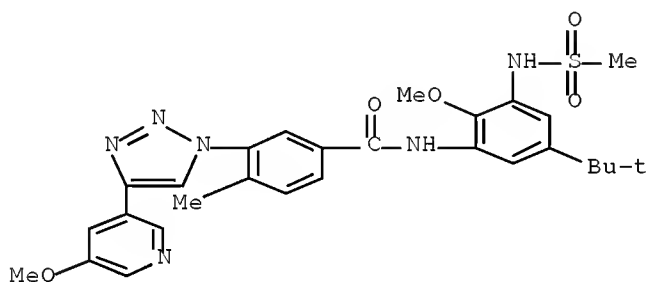
RN 865796-34-5 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-3-[4-(6-methoxy-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-4-methyl- (CA INDEX NAME)



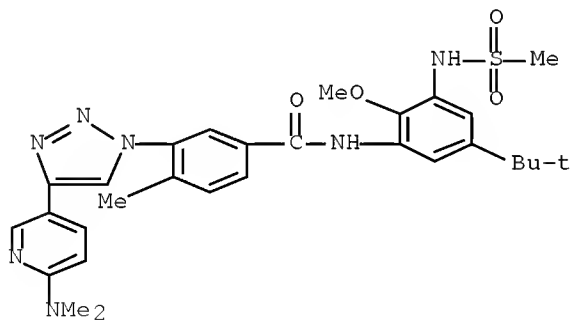
RN 865796-35-6 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-3-[4-(5-methoxy-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-4-methyl- (CA INDEX NAME)



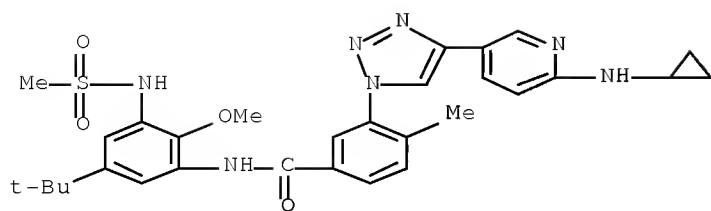
RN 865796-36-7 CAPLUS

CN Benzamide, 3-[4-[6-(dimethylamino)-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (CA INDEX NAME)



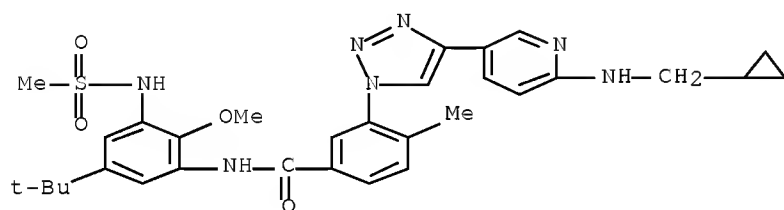
RN 865796-38-9 CAPLUS

CN Benzamide, 3-[4-[6-(cyclopropylamino)-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (CA INDEX NAME)



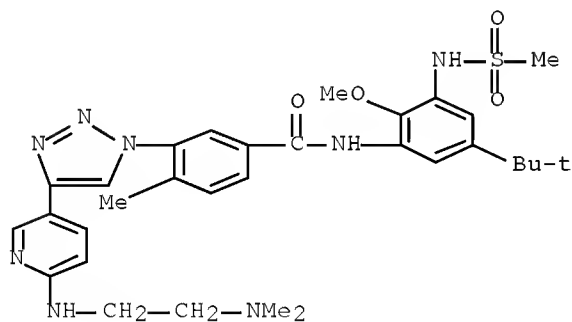
RN 865796-40-3 CAPLUS

CN Benzamide, 3-[4-[6-[(cyclopropylmethyl)amino]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (CA INDEX NAME)



RN 865796-50-5 CAPLUS

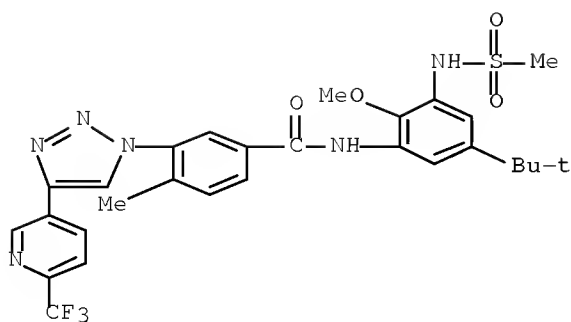
CN Benzamide, 3-[4-[6-[[2-(dimethylamino)ethyl]amino]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (CA INDEX NAME)



RN 865796-83-4 CAPLUS

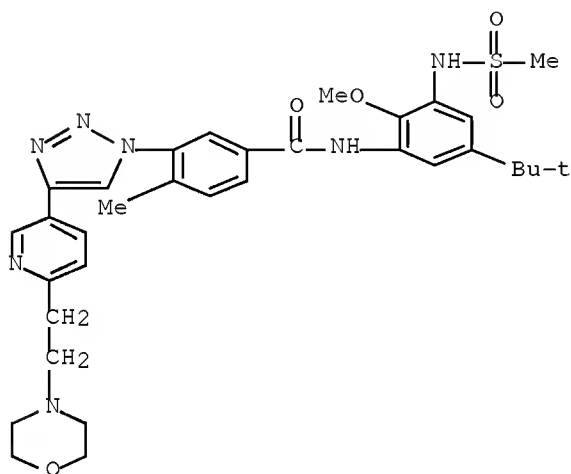
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-[6-(trifluoromethyl)-3-pyridinyl]-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)





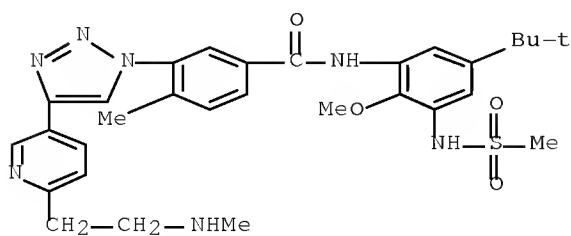
RN 865797-72-4 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-[6-[2-(4-morpholinyl)ethyl]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



RN 865797-73-5 CAPLUS

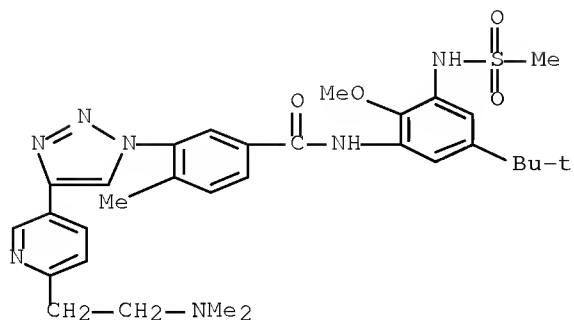
CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl-3-[4-[6-[2-(methylamino)ethyl]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



RN 865797-74-6 CAPLUS

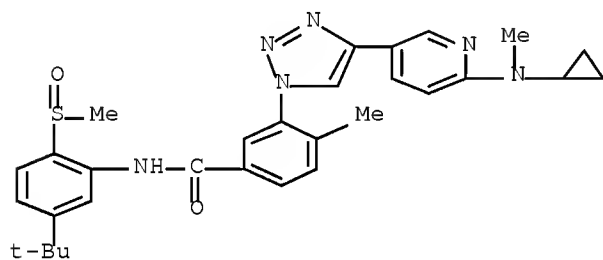
CN Benzamide, 3-[4-[6-[2-(dimethylamino)ethyl]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-

4-methyl- (CA INDEX NAME)



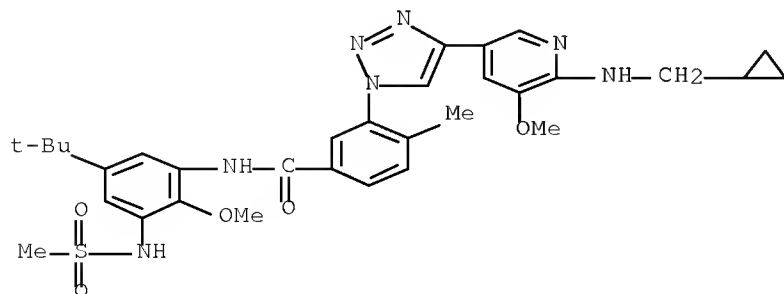
RN 865797-97-3 CAPLUS

CN Benzamide, 3-[4-[6-(cyclopropylmethylamino)-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-(methylsulfinyl)phenyl]-4-methyl- (CA INDEX NAME)



RN 865798-01-2 CAPLUS

CN Benzamide, 3-[4-[6-[(cyclopropylmethyl)amino]-5-methoxy-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-4-methyl- (CA INDEX NAME)



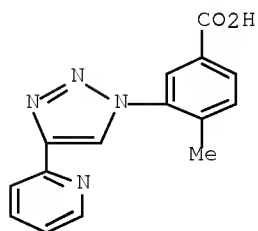
IT 865798-70-5 865798-72-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of triazolyl arylbenzamides as inhibitors of cytokines)

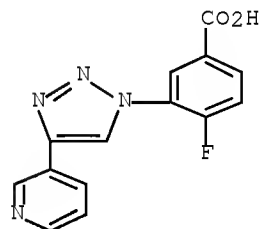
RN 865798-70-5 CAPLUS

CN Benzoic acid, 4-methyl-3-[4-(2-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



RN 865798-72-7 CAPLUS

CN Benzoic acid, 4-fluoro-3-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



IT 865798-05-6P 865798-09-0P 865798-10-3P

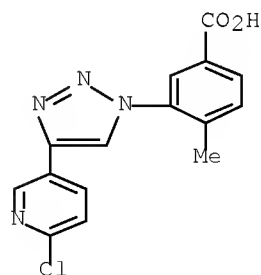
865798-11-4P 865798-68-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of triazolyl arylbenzamides as inhibitors of cytokines)

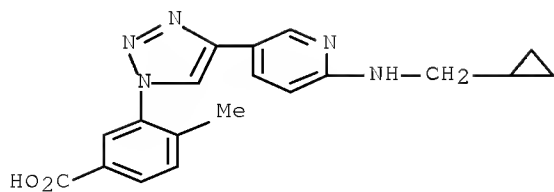
RN 865798-05-6 CAPLUS

CN Benzoic acid, 3-[4-(6-chloro-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-4-methyl- (CA INDEX NAME)



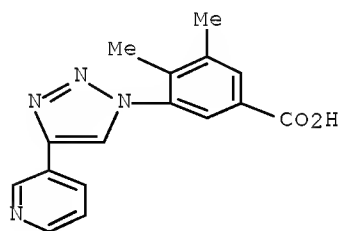
RN 865798-09-0 CAPLUS

CN Benzoic acid, 3-[4-[6-[(cyclopropylmethyl)amino]-3-pyridinyl]-1H-1,2,3-triazol-1-yl]-4-methyl- (CA INDEX NAME)



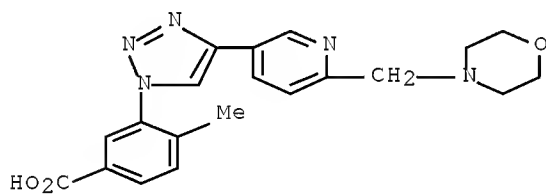
RN 865798-10-3 CAPLUS

CN Benzoic acid, 3,4-dimethyl-5-[4-(3-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



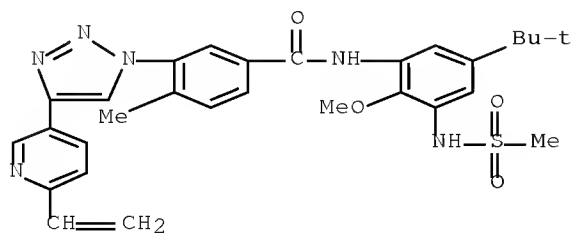
RN 865798-11-4 CAPLUS

CN Benzoic acid, 4-methyl-3-[4-[6-(4-morpholinylmethyl)-3-pyridinyl]-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



RN 865798-68-1 CAPLUS

CN Benzamide, N-[5-(1,1-dimethylethyl)-2-methoxy-3-[(methylsulfonyl)amino]phenyl]-3-[4-(6-ethenyl-3-pyridinyl)-1H-1,2,3-triazol-1-yl]-4-methyl- (CA INDEX NAME)



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(3 CITINGS)  
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2004:654838 CAPLUS Full-text

DOCUMENT NUMBER: 141:325154

TITLE: Discovery of Novel Heteroarylazoles That Are  
Metabotropic Glutamate Subtype 5 Receptor Antagonists  
with Anxiolytic Activity

AUTHOR(S): Roppe, Jeffrey; Smith, Nicholas D.; Huang, Dehua;  
Tehrani, Lida; Wang, Bowei; Anderson, Jeffrey;  
Brodkin, Jesse; Chung, Janice; Jiang, Xiaohui; King,  
Christopher; Munoz, Benito; Varney, Mark A.; Prasit,  
Petpiboon; Cosford, Nicholas D. P.

CORPORATE SOURCE: Merck Research Laboratories, San Diego, CA, 92121, USA

SOURCE: Journal of Medicinal Chemistry (2004),  
47(19), 4645-4648

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:325154

AB The highly potent, selective, and brain-penetrant metabotropic glutamate  
subtype 5 (mGlu5) receptor antagonists 3-(5-pyridin-2-yl-2H-tetrazol-2-  
yl)benzonitrile and 3-fluoro-5-(5-pyridin-2-yl-2H-tetrazol-2-yl)benzonitrile  
are reported. Compound 3-(5-pyridin-2-yl-2H-tetrazol-2-yl)benzonitrile is  
active in the rat fear-potentiated startle (FPS) model of anxiety with ED50 =  
5.4 mg/kg (po) when dosed acutely. In this model the anxiolytic effects of 3-  
(5-pyridin-2-yl-2H-tetrazol-2-yl)benzonitrile rapidly tolerate on repeated  
dosing.

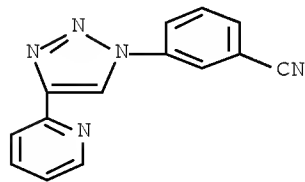
IT 550364-06-2F

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(discovery of novel heteroarylazoles that are metabotropic glutamate  
subtype 5 receptor antagonists with anxiolytic activity)

RN 550364-06-2 CAPLUS

CN Benzonitrile, 3-[4-(2-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 46 THERE ARE 46 CAPLUS RECORDS THAT CITE THIS  
RECORD (47 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:491005 CAPLUS Full-text

DOCUMENT NUMBER: 139:69268

TITLE: Preparation of heteroaryl substituted triazole derivatives as modulators of metabotropic glutamate receptor-5

INVENTOR(S): Cosford, Nicholas D. P.; Tehrani, Lida R.; Roppe, Jeffrey R.; Smith, Nicholas D.; Prasit, Petpiboon

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 55 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

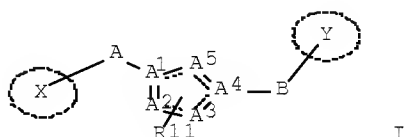
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051315	A2	20030626	WO 2002-US41720	20021213 <--
WO 2003051315	A3	20031023		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2469821	A1	20030626	CA 2002-2469821	20021213 <--
CA 2469821	C	20091020		
AU 2002366388	A1	20030630	AU 2002-366388	20021213 <--
AU 2002366388	B2	20080918		
EP 1458708	A2	20040922	EP 2002-805227	20021213 <--
EP 1458708	B1	20070926		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005516920	T	20050609	JP 2003-552248	20021213 <--
JP 4299139	B2	20090722		
AT 374194	T	20071015	AT 2002-805227	20021213 <--
ES 2292854	T3	20080316	ES 2002-805227	20021213 <--
WO 2004030637	A2	20040415	WO 2003-US9717	20030331 <--
WO 2004030637	A3	20040923		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003218462	A1	20040423	AU 2003-218462	20030331 <--
US 20050020585	A1	20050127	US 2004-499391	20040617 <--
US 7105548	B2	20060912		
PRIORITY APPLN. INFO.:				
			US 2001-341582P	P 20011218 <--
			WO 2002-US31294	A 20021001 <--
			WO 2002-US40147	A 20021213 <--
			WO 2002-US41720	W 20021213 <--
			WO 2002-US40237	A 20021216 <--
			WO 2002-US40486	A 20021217 <--

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 139:69268

GI



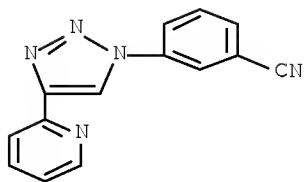
AB Triazole compds. substituted directly, or by a bridge, with a heteroaryl moiety containing N adjacent to the point of connection of the heteroaryl [I; X, Y = aryl or heteroaryl wherein at least one of X and Y is a heteroaryl with N adjacent to the position of attachment to A or B resp.; three of A1, A2, A3, A4, and A5 are N, the remaining are C, and one of A1 and A4 must be N, but not both A1 and A4 are N; X or Y is optionally substituted with 1-7 substituent groups wherein optionally two substituents are combined to form a cycloalkyl or heterocycloalkyl ring fused to X or Y; A is -C0-4 alkyl-, -C0-2-alkyl-SO-C0-2 alkyl-, -C0-2-alkyl-SO2-C0-2 alkyl-, -C0-2-alkyl-CO-C0-2 alkyl-, -C0-2 alkyl-NR9CO-C0-2 alkyl-, -C0-2 alkyl-NR9SO2-C0-2 alkyl- or -hetero C0-4 alkyl; B = -C0-4 alkyl-, -C0-2 alkyl-SO-C0-2 alkyl-, -C0-2 alkyl-SO2-C0-2 alkyl-, -C0-2 alkyl-CO-C0-2 alkyl-, -C0-2 alkyl-NR10CO-C0-2 alkyl-, -C0-2alkyl-NR10SO2-C0-2-alkyl-, or -hetero C0-4 alkyl-; R9, R10 = (un)substituted C0-6 alkyl, C3-7 cycloalkyl, heteroaryl, aryl; R11 = halogen, C0-6 alkyl, C0-6 alkoxy, O, :N(C0-4 alkyl), or N(C0-4 alkyl)(C0-4 alkyl) wherein any alkyl optionally is substituted with 1-5 substituent groups] are prepared These compds. are metabotropic glutamate receptor-subtype 5 (mGluR5) modulators and useful in the treatment of psychiatric and mood disorders such as, for example, schizophrenia, anxiety, depression, bipolar disorder and panic, as well as in the treatment of pain, Parkinson's disease, cognitive dysfunction, epilepsy, circadian rhythm disorders, drug addiction, drug abuse, drug withdrawal and other diseases. Thus, 2-(1H-1,2,4-triazol-3-yl)pyridine 1.0, K2CO3 1.88, and 1-chloro-3-fluorobenzene 0.89 g were stirred in 20 mL DMF at ambient temperature, and heated at 100° for 16 h to give, after workup and silica gel chromatog., 2-[1-(3-chlorophenyl)-1H-1,2,4-triazol-3-yl]pyridine. The compds. I had mGluR5 inhibitory activity as shown by IC50 values of 10 μM or better in the calcium flux assay and/or inhibition of >50% at 100 μM concentration in the phosphatidylinositol hydrolysis assay in mouse fibroblast Ltk cells expressing human GluR5 (human GluR5/L38-20 cells).

IT 550364-06-2P, 3-[4-(Pyridin-2-yl)-1H-1,2,3-triazol-1-yl]benzonitrile 550364-09-5P, 2-[1-(3-Chlorophenyl)-1H-1,2,3-triazol-4-yl]pyridine 550364-11-9P, 2-[1-(3,5-Difluorophenyl)-1H-1,2,3-triazol-4-yl]pyridine 550364-13-1P, 2-[1-[3-Fluoro-5-[(pyridin-2-yl)oxy]phenyl]-1H-1,2,3-triazol-4-yl]pyridine  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroaryl substituted triazole derivs. as modulators of metabotropic glutamate receptor-5 in treatment of psychiatric, mood disorders, and other diseases)

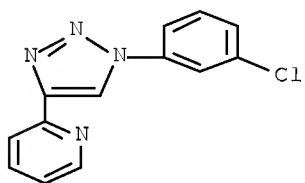
RN 550364-06-2 CAPLUS

CN Benzonitrile, 3-[4-(2-pyridinyl)-1H-1,2,3-triazol-1-yl]- (CA INDEX NAME)



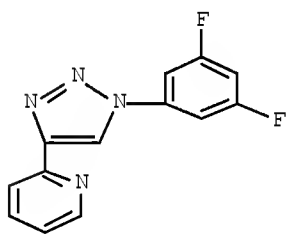
RN 550364-09-5 CAPLUS

CN Pyridine, 2-[1-(3-chlorophenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



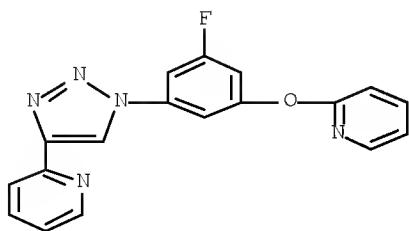
RN 550364-11-9 CAPLUS

CN Pyridine, 2-[1-(3,5-difluorophenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



RN 550364-13-1 CAPLUS

CN Pyridine, 2-[1-[3-fluoro-5-(2-pyridinyloxy)phenyl]-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11

THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS



L15 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2001:12273 CAPLUS Full-text

DOCUMENT NUMBER: 134:86271

TITLE: Preparation of pyrimidine derivatives as Src-family protein tyrosine kinase inhibitor compounds

INVENTOR(S): Armstrong, Helen M.; Beresis, Richard; Goulet, Joung L.; Holmes, Mark A.; Hong, Xingfang; Mills, Sander G.; Parsons, William H.; Sinclair, Peter J.; Steiner, Mark G.; Wong, Frederick; Zaller, Dennis M.

PATENT ASSIGNEE(S): Merck &amp; Co., Inc., USA

SOURCE: PCT Int. Appl., 470 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

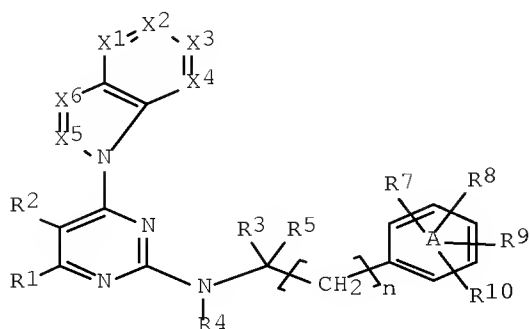
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000213	A1	20010104	WO 2000-US17443	20000626 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2383546	A1	20010104	CA 2000-2383546	20000626 <--
EP 1206265	A1	20020522	EP 2000-941701	20000626 <--
EP 1206265	B1	20031112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
US 6498165	B1	20021224	US 2000-604305	20000626 <--
JP 2003523942	T	20030812	JP 2001-505922	20000626 <--
AT 253915	T	20031115	AT 2000-941701	20000626 <--
PRIORITY APPLN. INFO.:				
			US 1999-141639P	P 19990630 <--
			WO 2000-US17443	W 20000626 <--

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 134:86271

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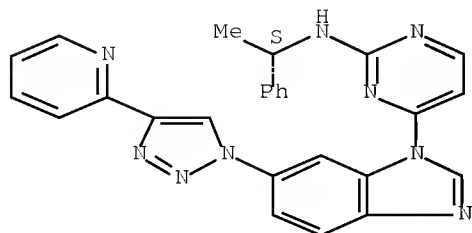
AB What are claimed are pyrimidine compds. (shown as I), or their pharmaceutically acceptable salts, hydrates, solvates, crystal forms and individual diastereomers, and pharmaceutical compns. including the same and their use as inhibitors of tyrosine kinase enzymes and consequently their use in the prophylaxis and treatment of protein tyrosine kinase-associated disorders, such as immune diseases, hyperproliferative disorders and other diseases in which inappropriate protein kinase action is believed to play a role, such as cancer, angiogenesis, atherosclerosis, graft rejection, rheumatoid arthritis and psoriasis. In I, R1, R2 = independently H, halo, OH, SH, CN, NO2, alkyl, alkoxy, acyloxy, alkoxycarbonyloxy, carbamoyloxy, alkylthio, sulfinyl, sulfonyl, acyl, alkoxycarbonyl, carbamoyl, amino, acylamino, ureido, sulfamoyl, sulfonylamino, or R1 and R2 can join together to form a fused methylenedioxy ring or a fused 6-membered aromatic ring; terms such as 'alkyl' here and below are further defined in the claims. R3, R5 = independently H, C1-C6-alkyl unsubstituted or substituted with 1-3 substituents, aryl, or R3 and R5 taken together can represent :O; R3 or R5 can represent a 2 or 3 C methylene bridge forming a ring of 5-8 atoms fused to the A ring. R4 = H, C1-C6-alkyl, C1-C6-alkoxyl. X1, X2, X3, X4 in -X1:X2-X3:X4- are substituted or unsubstituted CH or N where 0-2 of X1, X2, X3, X4 are N. X5, X6 = independently N, C, optionally substituted CH. A ring = Ph, naphthyl, pyridyl, pyrazinyl, pyrimidinyl, pyrrolyl, thienyl, oxazolyl, isoxazolyl, thiazolyl, pyrazolyl, triazolyl, tetrazolyl, furanyl, benzothienyl, benzofuranyl, indolyl, imidazolyl, benzimidazolyl, thiadiazolyl. R7, R8, R9, R10 = independently H, halo, OH, SH, CN, NO2, N3, N2+BF4-, alkyl, alkoxy, alkylthio, sulfinyl, sulfonyl, C1-C6-alkyl, C1-C6-perfluoroalkyl, acyl, alkoxycarbonyl, carbamoyl, acyloxy, alkoxycarbonyloxy, carbamoyloxy, amino, acylamino, ureido, sulfamoyl, sulfonylamino, two of R7, R8, R9, and R10 when on adjacent carbons join together to form a methylenedioxy bridge. N = 0-2. More than 500 example prepns. are given, but no preparative method is claimed and no data relating to the usefulness of the compds. are given. [This abstract record is one of 2 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 317826-55-4P, 2-[(S)-1-Phenylethylamino]-4-[6-(4-(pyridin-2-yl)-1,2,3-triazol-1-yl)benzimidazol-1-yl]pyrimidine  
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyrimidine derivs. as Src-family protein tyrosine kinase inhibitor compds.)

RN 317826-55-4 CAPLUS

CN 2-Pyrimidinamine, N-[(1S)-1-phenylethyl]-4-[6-[4-(2-pyridinyl)-1H-1,2,3-triazol-1-yl]-1H-benzimidazol-1-yl]- (CA INDEX NAME)

Absolute stereochemistry.



RECORD (17 CITINGS)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1998:68025 CAPLUS Full-text

DOCUMENT NUMBER: 128:180366

ORIGINAL REFERENCE NO.: 128:35595a,35598a

TITLE: Triazolines. XXXIII. Nonregiospecific  
1,3-cycloaddition of aryl azides to vinylpyridines: a  
unique route to the synthesis of 2-pyridyl substituted  
aziridines via unstable 4-pyridyltriazoline  
intermediates

AUTHOR(S): Lin, Zhaiwei; Kadaba, Pankaja K.

CORPORATE SOURCE: K and K Biosciences, Inc., Lexington, KY, 40502-3330,  
USA

SOURCE: Journal of Heterocyclic Chemistry (1997),  
34(6), 1645-1650

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER: HeteroCorporation

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:180366

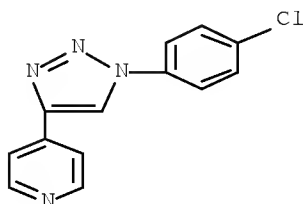
AB The 1,3-cycloaddn. of aryl azides to the olefinic bonds of 4- and 2-  
vinylpyridines was found to yield pyridyl-substituted aziridines as the main  
reaction products with only smaller amts. of the normally expected 1-aryl-5-  
pyridyl-1,2,3-triazolines. Theor. and exptl. evidence is provided to explain  
the results: based on the fact that the olefinic bonds in 4- and 2-  
vinylpyridines are electron-deficient, azide addition can be expected to be  
not regiospecific. In the bidirectional addition reaction, the HOMO(azide)-  
LUMO(olefin) interaction predominates leading to unstable 1-aryl-4-pyridyl-  
1,2,3-triazolines, which, unlike the more stable 5-pyridyl compds., lose  
nitrogen under thermal conditions to yield the aziridines. At room  
temperature, the reactions yield the aziridine along with the 1-aryl-4-  
pyridyltriazole, providing evidence for the formation of the 4-  
pyridyltriazoline intermediate. Reaction of the vinylpyridines with variously  
substituted Ph azides, clearly indicates that the electron donating Me and  
methoxy groups on the Ph azide facilitate reaction, while the electron  
withdrawing nitro group has a retarding effect. This is consistent with an  
increase in the HOMO(azide) energy and hence in azide reactivity. According  
to the FMO model, the 1,3-cycloaddn. of aryl azides to vinylpyridines appears  
to be predominantly, but not exclusively, a HOMO(azide)-LUMO(olefin)  
interaction and provides a unique route to the synthesis of 2-pyridyl  
substituted aziridines.

IT 191797-37-2F

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 191797-37-2 CAPLUS

CN Pyridine, 4-[1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)  
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1997:352799 CAPLUS Full-text

DOCUMENT NUMBER: 127:81400

ORIGINAL REFERENCE NO.: 127:15609a,15612a

TITLE: Triazolines 30. Nonregiospecific 1,3-cycloaddition of  
aryl azides to vinylpyridines: a unique route to  
pyridyl substituted aziridines

AUTHOR(S): Kadaba, Pankaja K.; Lin, Zhaiwei

CORPORATE SOURCE: Division of Medicinal Chemistry and Pharmaceuticals,  
College of Pharmacy, Chandler Medical Center,  
University of Kentucky, Lexington, KY, 40536-0082, USA

SOURCE: Heterocyclic Communications (1997), 3(2),  
163-168

CODEN: HCOMEX; ISSN: 0793-0283

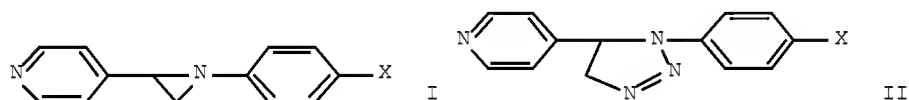
PUBLISHER: Freund

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:81400

GI



AB The 1,3-cycloaddn. of Ph azides 4-XC<sub>6</sub>H<sub>4</sub>N<sub>3</sub> (X = Cl, Me, NO<sub>2</sub>) to the olefinic double bond of 4-vinylpyridine, yields the 1-phenyl-2-pyridylaziridine I as the main product with only smaller amts. of the 1-phenyl-5-pyridyl-1,2,3-triazoline II, although the reaction constitutes a general approach to the synthesis of Δ<sup>2</sup>-1,2,3-triazolines. Exptl. and theor. evidence are provided to explain the results on the basis that the olefinic bond in 4-vinylpyridine is an electron-deficient bond and that azide addition is not regiospecific. In the bidirectional addition reaction, the HOMOazide-LUMOolefm interaction predominates leading to a 1-phenyl-4-pyridyl-1,2,3-triazoline, which, unlike the 5-pyridyl compound, loses nitrogen under thermal conditions to yield the aziridine, and at room temperature, a mixture of the resp. triazole and the aziridine.

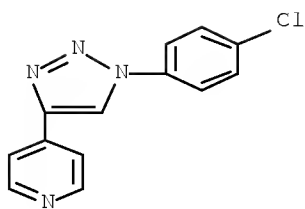
IT 191797-37-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of pyridyl triazolines and aziridines by cycloaddn. of aryl azides to vinylpyridnes)

RN 191797-37-2 CAPLUS

CN Pyridine, 4-[1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)  
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1995:228869 CAPLUS Full-text

DOCUMENT NUMBER: 122:290182

ORIGINAL REFERENCE NO.: 122:52899a,52902a

TITLE: Thermolysis of 4-heteroaryl substituted  
5-azido-1H-1,2,3-triazoles: competition between  
rearrangement and decomposition

AUTHOR(S): L'abbe, Gerrit; Vercauteren, Karin; Dehaen, Wim

CORPORATE SOURCE: Department of Chemistry, University of Leuven,  
Heverlee, 3001, Belg.

SOURCE: Bulletin des Societes Chimiques Belges (1994  
, 103(7-8), 321-7

CODEN: BSCBAG; ISSN: 0037-9646

PUBLISHER: Societe Chimique Belges

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 5-Azidotriazoles bearing a thiazole, benzothiazole or pyridine ring at the 4-position were synthesized and thermolyzed at 60°C. Whereas the 5-azido-4-(thiazol-2-yl)triazole decomposed with extrusion of nitrogen and formation of the triazene as the sole reaction product, the 5-azido-4-(benzothiazol-2-yl)triazoles furnished mixts. of the triazines and the tetrazoles. In the case of the 5-azido-4-(2-pyridyl)triazoles, the product distribution was found to depend strongly on the N-1 aryl substituent, favoring the tetrazole by increasing the electron-withdrawing capacity of this group.

IT 163071-42-9P 163071-43-0P 163071-44-1P

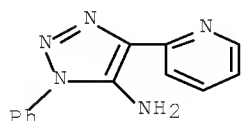
163071-45-2P 163071-46-3P 163071-47-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(thermolysis of heteroaryl-substituted azidotriazoles)

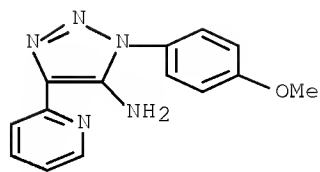
RN 163071-42-9 CAPLUS

CN 1H-1,2,3-Triazol-5-amine, 1-phenyl-4-(2-pyridinyl)- (CA INDEX NAME)



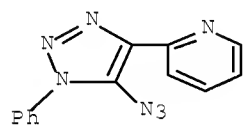
RN 163071-43-0 CAPLUS

CN 1H-1,2,3-Triazol-5-amine, 1-(4-methoxyphenyl)-4-(2-pyridinyl)- (CA INDEX  
NAME)



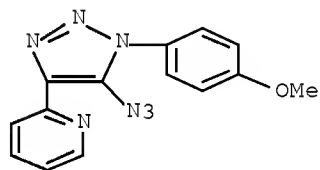
RN 163071-44-1 CAPLUS

CN Pyridine, 2-(5-amino-1-phenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



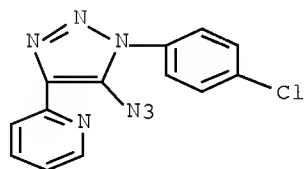
RN 163071-45-2 CAPLUS

CN Pyridine, 2-[5-azido-1-(4-methoxyphenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



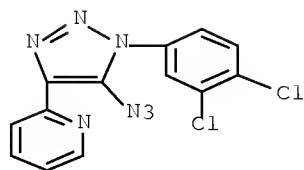
RN 163071-46-3 CAPLUS

CN Pyridine, 2-[5-azido-1-(4-chlorophenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



RN 163071-47-4 CAPLUS

CN Pyridine, 2-[5-azido-1-(3,4-dichlorophenyl)-1H-1,2,3-triazol-4-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD  
(3 CITINGS)

L15 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1979:611212 CAPLUS Full-text  
DOCUMENT NUMBER: 91:211212  
ORIGINAL REFERENCE NO.: 91:34025a

L15 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1977:189669 CAPLUS Full-text

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD  
(2 CITINGS)

L15 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN  
ACCESSION NUMBER: 1970:414768 CAPLUS Full-text  
DOCUMENT NUMBER: 73:14768  
ORIGINAL REFERENCE NO.: 73:2465a,2468a  
TITLE: Reactions of phenyl-2-pyridylglyoxals with hydrazines  
AUTHOR(S): Eistert, Bernd; Endres, Edmund  
CORPORATE SOURCE: Inst. Org. Chem., Univ. Saarlandes, Saarbruecken, Fed.  
Rep. Ger.  
SOURCE: Justus Liebigs Annalen der Chemie (1970),  
734, 56-69  
CODEN: JLACBF; ISSN: 0075-4617  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 73:14768

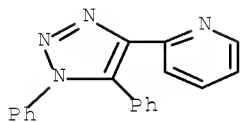
GI For diagram(s), see printed CA Issue.

AB Reaction of 2-(R-substituted)-3-(R1-substituted)-6-phenacylpyrimidines (I) with Br in the presence of AlCl3 and oxidation with Me2SO gave phenyl[2-(R-substituted)-3-(R1-substituted)-6-pyridyl]glyoxals (II) [where R = H or Me; R1 = H; or (RR1=)CH:CHCH:CH]. Reaction of II with R2NHNH2.H2O yielded the 2 possible N'-(R2-substituted)-monohydrazones (III and IV) of II (where R2 = H or p-MeC6H4SO2). Treatment of IV (R2 = H) with MnO2 yielded phenyl [6-(R1-substituted)-7-(R-substituted)-v- triazolo[1,5-a]pyrid-2-yl] ketones (V) [where R = H or Me; R1 = H; or (RR1 =)CH:CHCH:CH]. Reaction of V with PhNH2 in HOAc gave the corresponding 1,5-diphenyl-4-[6-(R-substituted)-5-(R1-substituted)-2-pyridyl]-1H-1,2,3- triazoles (VI).

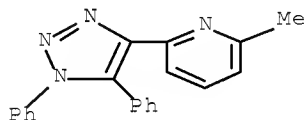
IT 27049-11-2P 27049-32-7P 27049-40-7P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 27049-11-2 CAPLUS

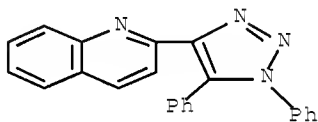
CN Pyridine, 2-(1,5-diphenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



RN 27049-32-7 CAPLUS  
 CN Pyridine, 2-(1,5-diphenyl-1H-1,2,3-triazol-4-yl)-6-methyl- (CA INDEX NAME)



RN 27049-40-7 CAPLUS  
 CN Quinoline, 2-(1,5-diphenyl-1H-1,2,3-triazol-4-yl)- (CA INDEX NAME)



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L15 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1959:34913 CAPLUS Full-text  
 DOCUMENT NUMBER: 53:34913  
 ORIGINAL REFERENCE NO.: 53:6266c-i,6267a  
 TITLE: 4-Aminoquinaldine compounds  
 INVENTOR(S): Jensch, Heinrich  
 PATENT ASSIGNEE(S): Farberke Hoechst AG vorm. Meister Lucius & Bruning  
 SOURCE: Addn. to Ger. 947,552 (preceding abstr.)  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

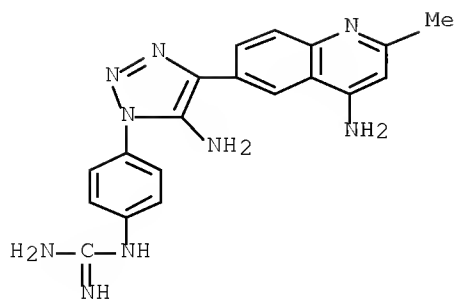
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 950637		19561011	DE 1944-F3788	19440527 <--

AB 4-Aminoquinaldine compds. are prepared by the following methods. (1) 4,6-Diaminoquinaldine or 6-aminoquinaldine containing a group in the 4-position convertible to an NH<sub>2</sub> group is condensed with guanidinobenzoyl halides. (2) N'-(4-Amino-6-quinaldyl)diaminocyanuric chloride substituted in the 4-position by a group convertible to an NH<sub>2</sub> group is condensed with an aminophenylguanidine. (3) (4-Amino-6-quinaldyl azide or a 6-quinaldyl azide containing a substituent in the 4-position convertible to an NH<sub>2</sub> group is condensed with a guanidinobenzyl cyanide. (4) (4-Amino-6-quinaldyl)acetonitrile or compds. substituted in 4-position by a group convertible to an NH<sub>2</sub> group is condensed with a guanidinophenyl azide. The



substituents in the 4-position are converted to the NH<sub>2</sub> group after the condensation. Thus, 20 g. p-aminobenzyl cyanide-HCl, 12 g. cyanamide, and 8 cc. H<sub>2</sub>O is heated on a water-bath, the clear melt diluted with H<sub>2</sub>O, alkalinized with concentrated NaOH, and cooled to give (p-guanidino)benzyl cyanide, m. 165-6° (decomposition) (H<sub>2</sub>O); HNO<sub>3</sub> salt, m. 189° (decomposition). Condensing of 1 mole free base with 1 mole 2-methyl-4-amino-6-quinolyl azide in alc. solution in the presence of 1 mole EtONa, refluxing the mixture 1 hr., cooling, and adding a little H<sub>2</sub>O yields 1-(2-methyl-4-amino-6-quinolyl)-4-(p-guanidinophenyl)-5-amino-1,2,3- triazole. (p-Aminophenyl)guanidine (I) carbonate (5 g.) is prepared by reducing (p-nitrophenyl)guanidine, m. 198-9° (decomposition), with H in the presence of Pd in AcOH, adding K<sub>2</sub>CO<sub>3</sub> and treating I carbonate, m. 180-1° (decomposition), with concentrated NaOH, or by warming p-aminoacetanilide-HCl with H<sub>2</sub>O and cyanamide, adding Na<sub>2</sub>CO<sub>3</sub>, recrystg. the formed (p-acetaminophenyl)guanidine carbonate from H<sub>2</sub>O, m. 220° (decomposition), and heating with dilute HCl with splitting off the Ac group. N'-(2-Methyl-4-amino-6-quinolyl)diaminocyanuric chloride (3.5 g.), and 100 g. H<sub>2</sub>O is refluxed 3 hrs., HNO<sub>3</sub> added, and the nitrate of N'-(2-methyl-4-amino-6-quinolyl)-N''-(p-guanidinophenyl)melamine converted to the free base by addition of NaOH. I carbonate (18.1 g.) is dissolved in 200 cc. H<sub>2</sub>O and 22 cc. concentrated H<sub>2</sub>SO<sub>4</sub>, diazotized with a solution of 7 g. NaNO<sub>2</sub> in 30 cc. H<sub>2</sub>O, a solution of 6 g. NaN<sub>3</sub> in 20 cc. H<sub>2</sub>O added with stirring and cooling, after complete reaction excess 2N HNO<sub>3</sub> added, and the precipitated (p-guanidinophenyl)azide nitrate (11.95 g.) recrystd. from H<sub>2</sub>O, m. 200° (decomposition); free base, recrystd. from H<sub>2</sub>O, m. 147-8° (decomposition). A solution of 2.3 g. Na in 150 cc. EtOH and 9.85 g. (2-methyl-4-amino-6-quinolyl) acetonitrile was refluxed 1 hr., cooled, the precipitate filtered off, washed with alc. and then with warm H<sub>2</sub>O, and recrystd. from alc. to give 1-(p-guanidinophenyl)-4-(2-methyl-4-amino-6-quinolyl)-5- (amino-1,2,3- triazole, decompose 245°. p-Aminobenzoic acid (16.2 g.), 8 cc. H<sub>2</sub>O, and 9.7 cc. concentrated HCl is mixed with 11.5 g. cyanamide, the thin paste warmed on the water-bath, the clear melt treated with sufficient amts. of dilute HCl, the solution cooled, the thick paste of (p-guanidino)benzoic acid-HCl filtered off, and washed with dilute HCl. Addition of Na<sub>2</sub>CO<sub>3</sub> solution yields a precipitate, insol. in dilute AcOH, readily soluble in NaOH, m. 280° (H<sub>2</sub>O) with vigorous foaming. The HCl salt is converted to (p-guanidino)benzoyl chloride-HCl, by refluxing with SOCl<sub>2</sub> during 0.5 hr. and removing the excess SOCl<sub>2</sub> in vacuo. Condensation with 4,6-diaminoquinoline in glacial AcOH, slight warming, dissolving the precipitated mass in H<sub>2</sub>O, and precipitating with NaOH yields 2-methyl-4-amino-6-[(p-guanidino)benzoylamino]quinoline, which may be recrystd. from H<sub>2</sub>O and alc.

IT 115122-77-5P, Guanidine,  
 [p-[5-amino-4-(4-amino-2-methyl-6-quinolyl)-1H-1,2,3-triazol-1-yl]phenyl]-  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 115122-77-5 CAPLUS  
 CN Guanidine, N-[4-[5-amino-4-(4-amino-2-methyl-6-quinolyl)-1H-1,2,3-  
 triazol-1-yl]phenyl]- (CA INDEX NAME)



=> D HIS

(FILE 'HOME' ENTERED AT 17:01:30 ON 11 MAR 2010)

FILE 'REGISTRY' ENTERED AT 17:02:23 ON 11 MAR 2010

L1 STRUCTURE UPLOADED  
 L2 13 S SSS SAM L1  
 L3 STRUCTURE UPLOADED  
 L4 6 S SSS SAM L3  
 L5 581 S SSS FULL L3  
 SAVE L5 HIRA10590586/A

FILE 'CAPLUS' ENTERED AT 17:08:14 ON 11 MAR 2010

L6 58 S L5  
 L7 17 S L6 AND (PY<2005 OR PRY<2005 OR AY<2005)  
 E US 200!-590586/APPS  
 E US200!-590586/APPS  
 E US2006-590586/APPS  
 L8 2 S E3  
 SEL RN L8

FILE 'REGISTRY' ENTERED AT 17:12:41 ON 11 MAR 2010

L9 557 S E1-E557  
 L10 74 S L9 AND L5  
 SAVE L10 TEMP HIR10590586/A

FILE 'CAPLUS' ENTERED AT 17:15:31 ON 11 MAR 2010

L11 4 S L10  
 L12 1 S L11 AND (PY<2005 OR PRY<2005 OR AY<2005)  
 L13 2 S L11 AND (PY<2006 OR PRY<2006 OR AY<2006)  
 L14 15 S L7 NOT L2  
 L15 16 S L7 NOT L13

=> LOGOFF Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	126.44	338.22
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-15.30	-15.30

STN INTERNATIONAL LOGOFF AT 17:24:52 ON 11 MAR 2010